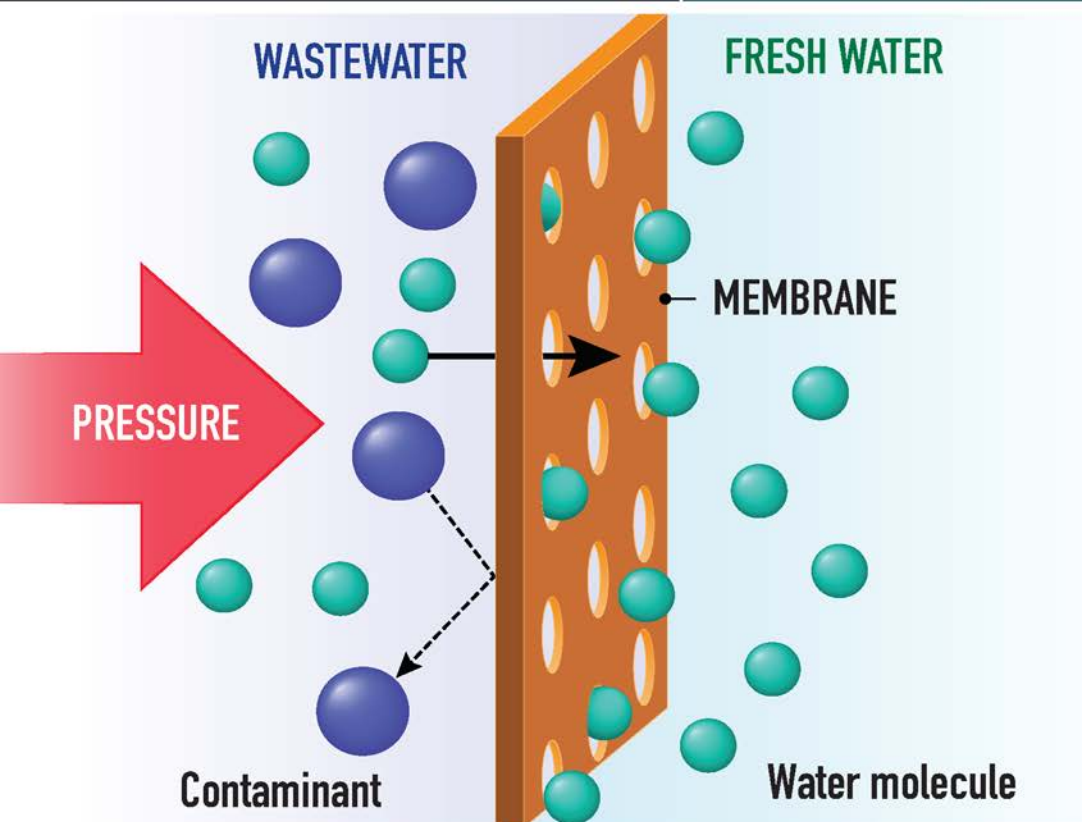


Wastewater Treatment by Reverse Osmosis Process

Mudhar Al-Obaidi
Chakib Kara-Zaitri
I. M. Mujtaba



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Contents

Preface.....	xv
Authors' Biographies.....	xxi

Chapter 1	Introduction	1
1.1	Introduction: Grand Challenges of the World	1
1.2	Wastewater.....	1
1.2.1	The Sources of Wastewater	2
1.2.2	Reused Water: Importance and Applications.....	2
1.2.3	Wastewater and Associated Challenges	3
1.3	Pollutants	4
1.3.1	Pollutants Complexity and Challenges.....	5
1.3.2	Phenolic Compounds.....	5
1.3.3	N-nitrosamine.....	6
1.3.4	Other Pollutants.....	7
1.3.4.1	Aniline (Amino Benzene).....	7
1.3.4.2	Acrylnitrile	7
1.3.5	Heavy Metals.....	8
1.4	Conclusions.....	8
	References	8

Chapter 2	Wastewater Treatment Methods	13
2.1	Introduction	13
2.2	Overview of Wastewater Treatment Methods	14
2.2.1	Physicochemical Treatment Methods.....	15
2.2.1.1	Coagulation and Flocculation.....	15
2.2.1.2	Activated Carbon Adsorption Method	16
2.2.2	Biological Treatment Methods	17
2.2.3	Advanced Treatment Methods	18
2.2.3.1	Advanced Oxidation Process.....	19
2.2.3.2	Limitations of Conventional Treatment Methods	21
2.2.4	Membrane Technology Treatment	21
2.2.5	Hybrid Systems	24
2.3	Conclusions.....	26
	References	27

Chapter 3	Membrane Processes	35
3.1	Introduction	35
3.2	Overview of Membrane Processes	35

3.3	Transport Mechanisms	36
3.4	Types of Pressure-Driven Membrane Processes	37
3.4.1	Nanofiltration (NF)	38
3.4.2	Reverse Osmosis (RO).....	38
3.5	RO Process Performance Measures	39
3.6	Types of RO Membrane Modules.....	40
3.6.1	Hollow Fibre Membrane Module	40
3.6.2	Spiral Wound Membrane Module.....	41
3.6.2.1	Characteristics of a Spiral Wound RO Process	41
3.6.2.2	Configuration of Spiral Wound Module.....	42
3.6.2.3	Limitations of RO Membrane Processes.....	42
3.7	Conclusions.....	45
	References	45

Chapter 4 Applications of Reverse Osmosis Process in Wastewater Treatment..... 49

4.1	Introduction	49
4.2	Historical Expansion of RO Use in Wastewater Treatment.....	49
4.3	Use of RO in Wastewater Treatment in Several Industrial Applications.....	50
4.3.1	Tannery Wastewater Treatment.....	51
4.3.2	Textile Wastewater Treatment	52
4.3.3	Electroplating Wastewater Treatment	54
4.3.4	Pharmaceutical Wastewater Treatment	54
4.3.5	Oily Wastewater Treatment.....	56
4.3.6	Pulp and Paper Wastewater Treatment.....	57
4.3.7	Dairy Wastewater Treatment.....	58
4.4	Use of RO in Small- to Large-Scale Wastewater Treatment Plants	60
4.4.1	Pilot-Scale Wastewater System	60
4.4.2	Large-Scale Wastewater System	61
4.4.2.1	Orange County Water District (OCWD): Groundwater Replenishment System in California.....	61
4.4.2.2	Ulu Pandan (UP) Wastewater Reclamation Plant in Singapore.....	61
4.4.3	Removal of Specific Pollutants From Wastewater Using RO Process.....	63
4.4.3.1	Heavy Metals	63
4.4.3.2	Arsenic.....	65
4.4.3.3	Cadmium	66
4.4.3.4	Chromium.....	66
4.4.3.5	Copper.....	68
4.4.3.6	Iron.....	68
4.4.3.7	Lead	69
4.4.3.8	Nickel.....	70

4.4.3.9	Mercury	71
4.4.3.10	Nitrogenous Compounds	71
4.4.3.11	Highly Toxic Organic Compounds	73
4.5	Conclusions.....	75
	References	75

Chapter 5	Modelling and Model Validation of Reverse Osmosis Process for Wastewater Treatment.....	87
5.1	Introduction	87
5.2	Modelling Rationale	89
5.3	RO Process Modelling Challenges.....	90
5.4	Membrane Transport Theories	90
5.4.1	Solution-Diffusion Model	90
5.4.2	Irreversible Thermodynamic Model	91
5.5	Overview of RO Process Modelling for Seawater and Brackish Water Desalination	93
5.6	Overview of RO Process Modelling for Wastewater Treatment.....	94
5.6.1	Model I: Al-Bastaki (2004)	95
5.6.1.1	Assumptions	95
5.6.1.2	Model Equations	96
5.6.1.3	Experimentation	98
5.6.1.4	Parameters Estimation (Determination of Transport Parameters)	99
5.6.1.5	Model Validation	99
5.6.2	Model II: Ahmad et al. (2007)	99
5.6.2.1	Assumptions	101
5.6.2.2	Model Equations	101
5.6.2.3	Experimentation	102
5.6.2.4	Parameters Estimation	103
5.6.2.5	Model Validation	103
5.6.3	Model III: Sagne et al. (2009)	104
5.6.3.1	Assumptions	105
5.6.3.2	Model Equations	105
5.6.3.3	Experimentation	107
5.6.3.4	Parameter Estimation	107
5.6.3.5	Model Validation	108
5.6.4	Model IV: Srinivasan et al. (2009, 2010).....	108
5.6.4.1	Assumptions	108
5.6.4.2	Model Equations	108
5.6.4.3	Experimentation	111
5.6.4.4	Parameter Estimation	112
5.6.4.5	Model Validation	112
5.6.5	Model V: Sundaramoorthy et al. (2011a).....	112
5.6.5.1	Assumptions	113
5.6.5.2	Model Equations	113

- 5.6.5.3 Experimentation 115
 - 5.6.5.4 Parameter Estimation 115
 - 5.6.5.5 Model Validation 116
- 5.6.6 Model VI: Fujioka et al. (2014) 116
 - 5.6.6.1 Assumptions 117
 - 5.6.6.2 Model Equations 117
 - 5.6.6.3 Experimentation 118
 - 5.6.6.4 Parameter Estimation 121
 - 5.6.6.5 Model Validation 121
- 5.6.7 Model VII: Al-Obaidi and Mujtaba (2016) 122
 - 5.6.7.1 Assumptions 123
 - 5.6.7.2 Model Equations 123
 - 5.6.7.3 Model Validation 127
- 5.6.8 Model VIII: Al-Obaidi et al. (2017b) 131
 - 5.6.8.1 Model Equations 131
 - 5.6.8.2 Parameter Estimation 134
 - 5.6.8.3 Model Validation 134
 - 5.6.8.4 Comparison of Performances by Using
Model VII and Model VIII 142
- 5.6.9 Model IX: Al-Obaidi et al. (2017c) 142
 - 5.6.9.1 Assumptions 142
 - 5.6.9.2 Model Equations 142
 - 5.6.9.3 Parameter Estimation Using the
gPROMS Software Suite 145
 - 5.6.9.4 Model Validation 147
- 5.6.10 Model X: Al-Obaidi et al. (2017d) 149
 - 5.6.10.1 Assumptions 149
 - 5.6.10.2 Model Equations 149
 - 5.6.10.3 Model Validation 151
- 5.6.11 Model XI: Al-Obaidi et al. (2018a) 151
 - 5.6.11.1 Parameters Estimation 155
 - 5.6.11.2 Model Validation 155
- 5.6.12 Model XII: Al-Obaidi et al. (2018b) 156
 - 5.6.12.1 Assumptions 156
 - 5.6.12.2 Model Equations 157
 - 5.6.12.3 Model Validation 158
- 5.6.13 Model XIII: Al-Obaidi et al. (2017e) 159
 - 5.6.13.1 Assumptions 159
 - 5.6.13.2 Model Equations 159
 - 5.6.13.3 Parameters Estimation 162
 - 5.6.13.4 Model Validation 162
- 5.6.14 Model XIV: Al-Obaidi et al. (2017f) 166
 - 5.6.14.1 Model Equations 166
 - 5.6.14.2 Parameter Estimation 168
 - 5.6.14.3 Model Validation 169

5.7	Critique on the Modelling of Spiral Wound Reverse Osmosis Process for Wastewater Treatment.....	171
5.8	Conclusions.....	172
	References	172

Chapter 6 RO Steady State and Dynamic Simulations for Wastewater

	Treatment.....	177
6.1	Introduction	177
6.2	The Importance of Simulation Studies.....	177
6.3	Overview of Steady State and Dynamic Simulations of RO Wastewater Treatment.....	178
6.4	Steady State Simulation: Sensitivity Analysis of the Operating Parameters	180
6.4.1	Removal of Copper From Electroplating Wastewater in Two RO Membranes	180
6.4.2	Removal of Copper and Nickel From Wastewater in a Laboratory-Scale RO Process	182
6.4.3	Removal of Methyl Orange Dye and Na ₂ SO ₄ Salt from Wastewater Using Spiral Wound RO Process	183
6.4.4	Removal of Ternary Solutes from Palm Oil Mill Effluents Using RO Process	185
6.4.5	Removal of Volatile Organic Molecules from Wastewater Using RO Process	186
6.4.6	Removal of Phenol from Wastewater in SG RO Membrane.....	186
6.4.7	Removal of Bisphenol A from Wastewater in Low-Pressure RO Process.....	190
6.4.8	Removal of Chlorophenol from Wastewater in an Individual Spiral Wound RO Process.....	193
6.4.8.1	Feed Flow Rate	193
6.4.8.2	Operating Pressure	201
6.4.8.3	Operating Concentration	203
6.4.9	Removal of Dimethylphenol from Wastewater in an Individual Spiral Wound RO Process.....	205
6.4.9.1	Sensitivity Analysis	205
6.4.10	Removal of Phenol from Wastewater in an Individual Spiral Wound RO Process	212
6.4.10.1	Sensitivity Analysis	212
6.4.11	Removal of Dimethylphenol from Wastewater in a Multi-Stage RO Process	217
6.4.11.1	Description of Multi-Stage RO Configurations	217
6.4.11.2	RO Network Performance Analysis	217

6.4.12	Removal of Nitrosamine from Wastewater in a Low-Pressure RO Process	223
6.4.12.1	Sensitivity Analysis of Operating Conditions	223
6.4.13	Removal of Nitrosamine from Wastewater in Full-Scale Multi-Stage RO Process.....	227
6.5	Dynamic Simulation: Sensitivity Analysis of the Operating Parameters	235
6.5.1	Removal of Multiple Solutes from a Palm Oil Mill Effluent Using RO Process.....	235
6.5.2	The Removal of Chlorophenol from Wastewater in an Individual Spiral Wound RO Process	239
6.5.2.1	Effect of Inlet Feed Pressure	239
6.5.2.2	Effect of Inlet Feed Flow Rate	242
6.5.2.3	Effect of Inlet Feed Concentration	244
6.5.3	Removal of Dimethylphenol from Wastewater in an Individual Spiral Wound RO Process.....	245
6.5.3.1	Inlet Feed Pressure	246
6.5.3.2	Inlet Feed Flow Rate.....	250
6.5.3.3	Inlet Feed Concentration	255
6.5.3.4	Inlet Feed Temperature.....	257
6.6	Conclusions.....	259
	References	259

Chapter 7	Optimisation of RO Process Superstructure for Wastewater Treatment.....	263
7.1	Introduction	263
7.2	Process Optimisation: Problem Formulation	264
7.3	Solution of RO Optimisation Problems.....	265
7.3.1	NLP-Based Optimisation	266
7.3.1.1	Successive Quadratic Programming technique.....	266
7.3.2	Superstructure Optimisation	267
7.4	Overview of the Superstructure Optimisation for an RO Processes-Based Wastewater Treatment	269
7.5	Optimal RO Network for the Removal of Two Chlorophenolic Compounds from Pulp Wastewater	270
7.6	Optimal RO Network for the Removal of Phenol from Wastewater of Lube-Oil Recycling Plants.....	273
7.7	Optimal RO Network for the Removal of Two Chlorophenolic Compounds from Pulp Wastewater Using an Advanced Optimisation Method.....	275
7.8	Minimisation of Freshwater Intake in a Petroleum Refinery	276

7.9	Minimisation of Freshwater Intake of Pulp and Paper Processes by Recycling and Regeneration of Wastewater Streams	277
7.10	Superstructure Optimisation of Water Network in a Petroleum Refinery.....	278
7.11	Superstructure Optimisation of the Pulp and Paper Industry Using Electrodialysis and RO Membranes Multi-Regenerator Systems	284
7.12	The Use of a Regenerated Water Network for Optimum Water Consumption in the Dairy Industry.....	287
7.13	Optimal RO Network Configuration for the Removal of Dimethylphenol from Wastewater.....	290
7.13.1	Optimisation Problem Description and Formulation	292
7.13.2	Optimisation Results and Discussion.....	293
7.14	Conclusions.....	294
	References	294

Chapter 8	Optimisation of an RO-Based Wastewater Treatment Process Using Genetic Algorithms.....	297
8.1	Introduction	297
8.2	General Concepts of Genetic Algorithm and Evolutionary Algorithms	297
8.2.1	Generalised Genetic Algorithm	297
8.2.2	Simple Genetic Algorithm	298
8.2.3	Non-Dominated Sorting Genetic Algorithm (NSGA).....	299
8.2.4	Species Conserving Genetic Algorithm (SCGA)	299
8.3	Application of Genetic Algorithms for Optimising an RO Desalination Process	305
8.4	Genetic Algorithm Optimisation of Several Industrial Wastewater Treatment Processes.....	306
8.5	Removal of Organic Pollutants from Wastewater Using GA Based Optimisation.....	308
8.5.1	Chlorophenol Removal from Wastewater	309
8.5.1.1	Optimisation Problem Description and Formulation.....	309
8.5.1.2	Genetic Algorithm Parameter Setting	310
8.5.1.3	Optimisation Results	312
8.5.2	N-nitrosodimethylamine (NDMA) Removal from Wastewater.....	314
8.5.2.1	Description of Permeate Reprocessing Multi-Stage RO Process.....	314

8.5.2.2	Optimisation Problem Description and Formulation.....	316
8.5.2.3	Optimisation Results	316
8.6	Conclusions.....	318
	References	318

Chapter 9	Recent Advances of Reverse Osmosis Design for Wastewater Treatment.....	321
9.1	Introduction	321
9.2	Advanced Design of Multi-Stage RO Process for the Removal of N-nitrosamine Compounds from Wastewater ...	321
9.3.1	Description of the Multi-Stage RO Process	322
9.3.2	Model XV.....	323
9.3.3	Sensitivity Analysis of the Operating Parameters	324
9.3.4	Optimisation of a Multi-Stage RO Process with ERD.....	330
9.3.4.1	Optimisation Problem 1 (OP1).....	330
9.3.4.2	Optimisation Problem 2 (OP2)	331
9.4	Advanced Design of a Two-Stage/Two-Pass Spiral Wound RO Process for the Removal of Chlorophenol from Wastewater.....	333
9.4.1	Two-Stage/Two-Pass RO Process	333
9.4.2	Sensitivity Analysis	335
9.4.3	Optimisation of the Two-Stage/Two-Pass Spiral Wound RO Process.....	335
9.5	Multi-Stage and Multi-Pass RO Networks for the Removal of N-nitrosodimethylamine-D6 from Wastewater.....	337
9.5.1	Multi-Stage Retentate Reprocessing Design of RO Process	337
9.5.1.1	Simulation of a Retentate Reprocessing Design of an RO Process	337
9.5.2	Multi-Stage Permeate Reprocessing Design of an RO Process	340
9.5.2.1	Simulation of a Permeate Reprocessing Design of an RO Process	340
9.5.3	Multi-Stage Multi-Pass Combined Permeate and Retentate Reprocessing of an RO Process	340
9.5.3.1	Simulation of Advanced Design of RO Process	342
9.5.4	Optimisation of Multi-Stage Multi-Pass Permeate-Retentate Reprocessing RO Process	342
9.5.4.1	Optimisation Results	343
9.6	Permeate and Retentate Stream Recycling of Multi-Stage RO Process for Chlorophenol Removal from Wastewater	344

9.6.1	Description of Multi-Stage Permeate and Retentate Streams Recycling of an RO Process.....	345
9.6.2	Simulation Results.....	345
9.6.2.1	Case Study 1	345
9.6.2.2	Case Study 2	348
9.6.3	Sensitivity Analysis of Operating Conditions	350
9.6.4	Impact of the Fresh Feed Flow Rate on the Performance of a Permeate Recycling RO Process ...	357
9.7	Design of a Multi-Stage RO Process for the Removal of Chlorophenol from Wastewater.....	361
9.7.1	Description of the Multi-Stage RO Process	361
9.7.2	Sensitivity Analysis of Operating Conditions	362
9.8	Design and Optimisation of the Membrane Element of a Spiral Wound RO Process for Dimethylphenol Removal from Wastewater at Low Energy Consumption	370
9.8.1	Effect of Membrane Width and Length	371
9.8.2	Effect of Feed Channel Height.....	372
9.8.3	Optimisation of Membrane Design Parameters.....	372
9.9	Design and Optimisation of Membrane Elements of a Multi-Stage RO Process for the Removal of Chlorophenol from Wastewater with Significant Energy Savings.....	373
9.9.1	Description of the RO Process and Feed Characteristics	376
9.9.2	Impact of Membrane Dimension on the Process Performance	377
9.9.3	Impact of Changing the Height of the Feed Channel	378
9.9.4	Impact of Membrane Area	378
9.9.5	Impact of Increasing the Membrane Area by Simultaneously Increasing Membrane Length and Width	381
9.9.6	Optimisation of RO Process Configurations with and without an ERD.....	381
9.10	Conclusions.....	385
	References	385

Chapter 10 Economic Aspects of RO Process for Wastewater Treatment 389

10.1	Introduction	389
10.2	State of the Art of Economic Aspects of Water and Wastewater RO Treatment Processes	390
10.3	Variables Affecting the Water Production Cost of an RO Wastewater Treatment	400
10.4	Cost Evaluation of RO Water Treatment Plants	401
10.5	Cost Analysis of RO Process for the Purification of Olive Mill Wastewater.....	402

10.5.1 RO Process Description402

10.5.2 Economic Analysis.....402

10.6 Cost Analysis of an RO Process for the Reclamation
of Dairy Wastewater.....404

10.6.1 RO Process Description404

10.6.2 Economic Model of Sethi and Wiesner (2000).....404

10.6.3 Economic Results.....405

10.7 Economic Simulation and Optimisation of Chlorophenol
Removal from Wastewater.....406

10.7.1 Process Model Development407

10.7.2 Sensitivity Analysis of Operating Conditions407

10.7.3 Multi-Objective Optimisation of the RO Process 415

10.7.3.1 Optimisation Results 418

10.7.4 Optimum Operating Conditions for Maximising
Chlorophenol Rejection..... 419

10.8 Conclusions.....420

References420

Index425

Preface

Water affects all facets of life for humans, animals, plants, and the environment. Without it, there would be no vegetation on land, no oxygen for animals to breathe, and no humans to survive. Water is an essential component of nearly everything we eat and drink now and into the future. Despite the fact that there are a variety of water sources, such as rivers, lakes, and groundwater, fresh drinking water only constitutes 3% of the total global water available. The increasing demand for fresh water in this heavily populated world and the continuously changing ecological environment due to greenhouse effects continue to pose a real and serious challenge.

As the world population grows, the heavily industrialised world we live in or strive to live in continues to generate vast volumes of wastewater plagued with industrial effluents, sewage, and many harmful, some carcinogenic, by-products, which are more often than not simply disposed of in rivers and oceans. The demand for even cleaner potable water will grow exponentially, and the need for high-quality water recycling and treatment will become even more prominent than ever before. This will be aggravated further by many droughts, which will not be limited to water-scarce regions of the world. Water shortages, even in the Western world, are set to push water recycling and treatment very high on the agenda of politicians and industrialists alike.

The treatment of wastewater by removing such harmful compounds, however, is neither cheap nor easy to do. There is therefore a clear and urgent need for more intensive research in wastewater treatment that is practical and achievable at the lowest possible cost. The most promising technology that can achieve this is that of reverse osmosis (RO). The aim of this book is to provide the state of the art for reverse osmosis with all its facets and associated technologies in the context of wastewater treatment.

Wastewater effluents of many industrial applications contain a variety of micropollutants, which are released into a variety of water resources. Such micropollutants not only disrupt the biological ecosystem, but they also pose a real threat to the water supply for human consumption and to aquatic ecosystems. This book starts by discussing different organic compounds found in the wastewater of several industrial applications and raises awareness about increased and tighter legislation. Broadly speaking, the existence of even a trace amount of such highly toxic compounds in industrial effluents can prohibit the reuse of water in many applications.

Much attention has already been paid by health agencies around the world to establish tight targets for removing these harmful pollutants from industrial effluents before discharging them to surface water. For example, the United States Environmental Protection Agency (US EPA) has classified phenolic compounds as highly toxic compounds. The Agency of Toxic Substances and Disease Registry (ATSDR) limited the concentration of dimethylphenol to a maximum of 0.05 ppm in surface water. This particular harmful compound has the ability to remain in the environment for a long time. The World Health Organization (WHO) has set the phenol concentration to 1 µg/l in drinking water. Water UK regulators have set

the maximum concentration of phenol in the discharge wastewater of hospitals to be within 10 ppm, whereas the European Union (EU) has regulated total phenols in drinking water to be less than 0.0005 ppm. The environmental legislated value of 0.5 ppm of phenol has now been adopted before discharging the effluents into sewage system.

N-nitrosamine (especially NDMA, N-nitrosodimethylamine-D6) is one of the most toxic compounds found in wastewater, and rates above legal limits have been found in treated water supply systems including drinking water and wastewater facilities. Therefore, many water authorities around the globe are now regulated against a strict allowable N-nitrosamine concentration level in drinking water and recycled water. The International Agency for Research on Cancer has classified N-nitrosamine as a carcinogenic compound to humans where a cancer risk level is exhibited at 0.7 ng/L concentration. The US Environmental Protection Agency has restricted the concentration of N-nitrosamine in recycled water to this same level. Because of the high severity of harm caused by the compound, this book provides a thorough investigation into the latest methodologies for removing N-nitrosamine and similar compounds from wastewater.

With the increasing depletion of water resources around the world, there has never been a more urgent requirement to gain a deeper understanding of the aggressive contamination levels in a variety of wastewaters. There is an equally urgent requirement for sustainable filtration technologies capable of removing harmful substances, even at low concentration, from wastewater and therefore ceasing dependence on freshwater sources.

This book discusses the aforementioned two challenges in some detail. Technologies highlighted include physicochemical, biological, and advanced treatments such as membrane filtration technology and hybrid systems. Both theory and practice have indicated that the most efficient technologies are those which combine two or more treatment technologies, such as coagulation with ferric chloride, disinfection by chloramination, ultrafiltration (UF), reverse osmosis (RO), and ultraviolet radiation-hydrogen peroxide advanced oxidation process UV/H₂O₂. However, with the exception of reverse osmosis, all such advanced technologies require high energy and are therefore expensive. Reverse osmosis not only yields a much cheaper solution in terms of energy consumption, but it also delivers water quality commensurate with the ever increasingly stringent limits of high-toxic compounds concentration.

Reverse osmosis technology was initially used for the desalination of seawater and brackish water to produce drinking water. However, its rapid growth in various applications has transformed it into a commercially viable solution for treating and removing industrial effluents from wastewater. Advanced membrane technology with reverse osmosis is now recognised as the most promising technology for water recycling and reuse, due to its ability to achieve low levels of pollutant concentration in the permeate, and to therefore reclaim good-quality water for yet more applications. Having said this, the removal of high toxicological organic compounds from wastewater poses various complex challenges, which are explored in detail in this book.

This book discusses several studies using reverse osmosis for the removal of phenolic and N-nitrosamine compounds and other highly toxic compounds from wastewater. Such studies include several simulation and experimental methodologies. The

research described in this book readily confirms that much more work is still needed for optimising existing rigorous models. The book also explores other attempts, including distributed spiral wound reverse osmosis process models used especially for wastewater treatment.

The book covers the state of the art for the RO process and 10 RO process models of different features and complexities.

The first half of the book consists of five chapters.

- Chapter 1 briefly discusses grand challenges of the world including water. It discusses sources of wastewater, associated challenges, and the importance of water recycling. It highlights different types of pollutants in wastewater.
- Chapter 2 highlights different types of physicochemical and biological wastewater treatment methods including hybrid systems.
- Chapter 3 provides an overview of membrane processes and focusses on different types of membrane processes for water treatment, including nano-filtration and reverse osmosis. Different types and characteristics of membrane modules are also discussed.
- Chapter 4 gives a detailed overview of the application of RO process in different industries producing wastewater. It also highlights the application of RO in pilot-scale and large-scale wastewater treatment plants.
- Chapter 5 introduces the importance of process modelling for simulation, design, and optimisation. It highlights the challenges in RO process modelling, describes different membrane transport processes. The chapter provides a detailed account of 10 different types of RO process models used for evaluating and optimising the RO-based processes for wastewater treatment. The chapter also provides validation of each model using experimental data from literature.

The book provides detailed simulation of RO processes using the models presented in Chapter 5 and associated methods used for reducing the required energy consumption. These include optimising the operating conditions, extending the number of stages and module configurations, and implementing energy recovery devices (ERD) and membrane types. The book clearly shows that whilst significant enhancements have already been achieved in this area of work, substantial improvement can still be made to optimise all the operating conditions, which will yield the fastest, cheapest, and most sustainable solution. To this extent, the book discusses the merits of a multi-stage RO wastewater system for permeate and retentate recycling, two-pass configuration, reverse osmosis–catalyst wet air oxidation hybrid system, and superstructure optimisation for the removal of high-toxic compounds from wastewater. To this extent, the book also discusses an innovative optimisation method based on genetic algorithms for optimising a distributed model in a spiral wound RO process for the removal of organic compounds such as chlorophenol.

The minimisation of energy cost required for seawater desalination continues to be one of the main challenges in this area of work. This book explores several attempts for using multi-stage RO processes for the removal of highly toxic compounds from wastewater.

Against this backdrop, the book discusses in detail the state-of-the-art model-based techniques for removing highly toxic compounds from wastewater. Such models include those already validated against experimental research published in the last decades. The book essentially provides a one-stop shop for RO process operations including various rigorous methods for process modelling, simulation, and optimisation at the lowest energy cost, as well as advanced tools such as genetic algorithms (GA) for achieving the same. Where possible, the book provides illustrative examples of the various model-based simulation and optimisation studies used to explore several conceptual designs of multi-stage and multi-pass reverse osmosis processes. It is expected that this book will provide a detailed insight into practical sustainable solutions for removing harmful organic compounds from wastewater at low cost.

The second half of the book consists of five chapters.

- Chapter 6 highlights the importance of simulation studies and provides an overview of steady state and dynamic simulations of RO processes for wastewater treatment. It provides detailed examples of removing many toxic pollutants (from copper, dyes, volatile organic compounds, and phenolic compounds to nitrosamines).
- Chapter 7 describes in detail the optimisation of RO process superstructure for wastewater treatment. Detailed examples include cases from the pulp and paper, lube oil recycling, petroleum refining, and dairy industries.
- Chapter 8 introduces the concept of genetic algorithms (different types) for process optimisation. It provides the state-of-the art GA method in terms of its application in water desalination and wastewater treatment. The examples include removal of phenolic compounds and nitrosamines.
- Chapter 9 provides a detailed account of designing RO process for wastewater treatment. It highlights advanced design of multi-stage multi-pass RO process for removing nitrosamines and phenolic compounds from wastewater. This chapter also highlights the use of permeate and retentate reprocessing strategies for enhanced removal of pollutants from wastewater. Finally, optimisations of membrane module design (dimension) and feed channel design (dimension) are presented.
- Chapter 10 focusses on economic aspects of RO processes for wastewater treatment. It presents in detail several cost function models for evaluating different cost components (capital, operating, maintenance, labour, etc.) of RO processes. Examples are provided with reference to removing phenolic compounds from wastewater and reclaiming dairy wastewater.

A. SHORT DESCRIPTION

This book provides a one-stop shop for reverse osmosis, outlining its scope and limitations for the removal of organic compounds from wastewater. It starts by highlighting the challenges posed by a significant increase in demand of fresh water and the urgent need to recycle wastewater at minimum cost. It then addresses the

complexities of removing pollutants together with advantages and limitations of different conventional treatment methods. The reverse osmosis process is then presented in considerable detail, including process operation and feasibility for wastewater treatment. The book then presents the state of the art in respect of process modelling (steady state, dynamic, lumped, and distributed) for wastewater treatment. Current feasible solutions are discussed concerning their amenability for improving process performance and energy consumption based on process simulation using a wide range of operating parameters. Process improvement is achieved at optimised operating parameters and module dimensions and at the lowest energy consumption given the constraints set by the manufacturer's specification. The book then discusses the latest technologies in reverse osmosis, including the use of genetic algorithms, process hybridisation with the oxidation process presented for the first time, and lastly the economic aspect of the reverse osmosis process, more particularly for the removal of phenolic compounds from wastewater.

B. UNIQUE FEATURES

This book provides extensive technical coverage of the following key aspects:

1. Wastewater, reused water, and pollutant complexity.
2. Overview of wastewater treatment methods.
3. Membrane technology and critical analysis of the RO process.
4. Feasibility of the RO process in wastewater treatment.
5. RO process-based wastewater treatment modelling (simple to detailed).
6. RO process simulation for the removal of highly toxic compounds.
7. Steady state and dynamic behaviours of RO process in wastewater treatment and the sensitivity of unit performance based on a variety of operating parameters.
8. Wastewater RO network synthesis and network optimisation.
9. Implementation of genetic algorithm for optimising the RO process to maximise the removal of organic compounds from wastewater.
10. Advanced design of RO process using model-based optimisation techniques towards the removal of highly toxic compounds from wastewater.
11. RO process optimisation to increase process performance and reduce energy consumption.
12. Enhancement of individual and multi-stage RO process performance by optimising the process design parameters.
13. Exploring predictive designs of multi-stage and multi-pass RO process of high rejection.
14. Evaluation of the permeate reprocessing design in multi-stage RO-based wastewater treatment.
15. RO economics for water desalination with a precise focus on wastewater treatment.
16. Optimisation of product unit cost and total annual cost of chlorophenol removal from wastewater.



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1 Introduction

1.1 INTRODUCTION: GRAND CHALLENGES OF THE WORLD

Water affects all facets of life for humans, animals, plants, and the environment. Without it, there would be no vegetation on land, no oxygen for animals to breathe, and no humans to survive. Water is an essential component of nearly everything we eat and drink now and into the future. Even though there are a variety of water sources, such as rivers, lakes, and groundwater, fresh drinking water only constitutes 3% of the total global water available (Bielik et al., 2010). The increasing demand for fresh water in this heavily populated world and the continuously changing ecological environment due to greenhouse effects continue to pose a real and serious challenge. This is aggravated further with droughts, which are not limited to water-scarce regions of the world. In other regions of the world, where there is a shortage of drinking water, desalination water systems are used as they offer a technologically and economically viable solution (Kharraz et al., 2012; Droogers et al., 2012).

As the world population grows, the heavily industrialised world we live in continues to generate vast volumes of wastewater. This is, more often than not, plagued with industrial effluents, sewage, and many harmful, some carcinogenic, by-products, which are often disposed of in rivers and oceans. These contain heavy metals (Nyamayedenga, 2018) with highly toxic hydro-soluble metal ions and are major causes of environmental pollution. At the same time as this, there is a growing awareness of the impact of industrial effluents on wellbeing, health, and the ecosystem. With freshwater resources being depleted at a fast rate, it is clear that the demand for cleaner potable water is set to increase exponentially in future years, and the demand for high-quality water recycling and treatment will become even more prominent than ever before (Mujtaba et al., 2017, 2018). This is why there has been a surge of attempts to develop more cost-effective water treatment technologies. Many such attempts have focussed on treating wastewater to provide potable water at economical rates (Henze et al., 2008). The reused water from treated wastewater is one of the prominent sources of water being used in agriculture, municipalities (Levine and Asano, 2004; Jiménez and Asano, 2008), dairy and food industries (Buabeng-Baidoo et al., 2018), and power plants.

1.2 WASTEWATER

The fast-growing population and the associated increase in industrialisation have led to a significant increase of wastewater containing harmful industrial effluents and sewage. Such wastewater is, more often than not, disposed of in large volumes into surface water (Wade Miller, 2006; Henze et al., 2008; Mujtaba et al., 2018). The net effect of this is water pollution with abundant synthetic and geogenic organic compounds.

1.2.1 THE SOURCES OF WASTEWATER

Both the allowable quantity and quality of wastewater are dependent on the underlying industry it serves as well as the standards and regulations for that particular country. One hundred forty million tonnes of fertilisers and several million tonnes of pesticides are used globally each year. Unsurprisingly, Schwarzenbach et al. (2006) reported that 300 million tonnes of synthetic compounds are disposed annually into natural waters, and this number is rising. To deal with this problem, several attempts have been made to develop sustainable alternative methods such as recycling, reclaiming, and reusing of different types of wastewater.

1.2.2 REUSED WATER: IMPORTANCE AND APPLICATIONS

The terms reused, recycled, and reclaimed water are used for different sources of water which include industrial wastewater, municipal water, agricultural return flows, and poor-quality well water. Water reuse is on the increase even in countries with little or no water shortage (Wade Miller, 2006), and this has contributed to reducing the quantity of wastewater being dumped into water sources. Water reuse can also alleviate the problems of (a) freshwater shortages, especially in communities with high demand, (b) water depletion, and (c) groundwater contamination. The expectation nowadays is that water recycling will increasingly become one of the most efficient resources of high-quality water.

A survey taken by the Australian Academy of Technological Sciences and Engineering confirmed, according to Radcliffe (2004), reported that a total of 43.91 billion gallons per year (bgy) of water was reused in 2001–2002 in Australia, compared to 29.83 bgy used during 1996–1999. Similarly, a growing practice of water reuse in several European Union countries was reported in another survey conducted by the Water Reuse Foundation for the Global Water Research Coalition in 2004 (Bixio et al., 2006), indicating over 200 water reuse projects in Europe.

A variety of industrial and agricultural applications use reclaimed and reused waters due to the continuously increasing water demand (Beltrán and Koo-Oshima, 2006). This is because such applications only require low-quality water for irrigation. Thus, a significant amount of recycled water is used to irrigate edible and non-edible agricultural crops. This in turn reduces the consumption of fertilisers due to the high nutrient content and low cost of wastewater. Low-quality reused water is also used in cooling towers and power plants. Table 1.1 shows several examples of different countries which have used recycling/reclaiming water in different applications (as reported by Jiménez and Asano, 2008).

Water reuse networks have been emerging globally for the last 50 years. Wilcox et al. (2016) reviewed the economic, social, and environmental issues related to implementing water reuse networks in cities. Manufacturing industries are the major users of reclaimed water. Cooling and process water recycling accounts for around 30% of all water reuse applications (Van der Bruggen, 2010). The distance between industries and urban areas offers opportunities for the recycling of municipal wastewater in a variety of industrial applications.

TABLE 1.1
Implementation of Reclaimed and Recycled Wastewater in Different Countries

Country	Purpose	Rate	Notes
Pakistan	Agricultural	96%	Non-treated wastewater
Tunisia	Agricultural	86%	Treated wastewater
Germany	Industrial	69%	Germany and USA have the largest number of recycling and reuse projects for several industrial applications
USA	Industrial	45%	
Singapore	Municipal	45%	Singapore and Namibia have the largest water reuse from municipal projects
Namibia	Municipal	29%	

(Adapted from Jiménez and Asano, 2008)

Industrial water reuse can be enhanced by increasing wastewater discharge taxes, requiring the gradual use of alternative water sources, and encouraging the development of technologies capable of removing a wider range of contaminants than does conventional wastewater treatment (Van der Bruggen, 2010). But many small-scale industries can still find it difficult to have sustainable stand-alone water supplies due to heavy economic and environmental penalties.

An interesting initiative, often known as eco-industrial parks (EIP), has emerged in areas where there is a cluster of industries/plants within a confined geographic proximity and who share wastewater treatment processes to reduce costs (Alnouri et al., 2017; Fadzil et al., 2018).

There is little doubt that the level of implementation of municipal wastewater reclamation and industrial effluents reuse is set to increase in the future.

1.2.3 WASTEWATER AND ASSOCIATED CHALLENGES

Substantial amounts of wastewater effluents and sewage are disposed into rivers, lakes, and groundwater and severely affect human health and the natural ecosystem. For example, endocrine-disrupting chemicals (EDCs) are found in wastewater, surface water, and groundwater. Some of the known EDCs include agricultural chemicals such as pesticides, fungicides, and dioxins; phthalates such as butyl benzyl phthalate and diethyl phthalate; biphenyls such as bisphenol A; pharmaceutical drugs such as tamoxifen; and steroid estrogens such as the natural sex hormones estrone (E1) and 17β-estradiol (E2) and the synthetic hormone 17α-ethinyl estradiol (EE2) (Tizaoui et al., 2017). These EDCs can very easily get into water sources and can be the cause of adverse effects on humans and aquatic life (Tizaoui et al., 2017).

A considerable amount of research can be found in the literature on the recycling and reclaiming of wastewater with an efficient removal of micropollutants from wastewater. However, this is no small challenge because these highly toxic organic

pollutants found ubiquitously in wastewater are neither easily nor cheaply removed. Mujtaba et al. (2018) reviewed a number of such wastewater treatment processes.

Henze et al. (2008) confirmed that wastewater treatment is a much more difficult process compared to seawater desalination, mostly due to the existence of the complex toxicological compounds in wastewater and the requirement to use advanced and integrated technologies to remove them. In this respect, Hendricks (2006), Bolong et al. (2009), and Mujtaba et al. (2018) have reviewed several challenges associated with the removal of micropollutants from wastewater. These are summarised below:

- Several types of organic compounds can be found in wastewater. These increase the possibility of forming high toxicological compounds as a result of chemical reactions.
- The establishment of a unique guideline of restricted concentration for new organic high-toxicity compounds such as N-nitrosamine in wastewater is not agreed yet.
- The list of contaminants found in wastewater has increased to now include synthetic organics and countless disinfection by-products.
- Some highly toxic organic compounds at a very low concentration (nanograms per litre), but still harmful, have been traced in the secondary treatment process of effluents. These would require complex and effective analytical techniques because of the very low concentration rates of contaminants.
- Increased knowledge of pollutants and their ecological and health effects has tightened the already stringent rules by requiring the removal of disinfection by-products.

The necessity to explore all feasible solutions for wastewater treatment methods for reducing contaminant concentrations is clear. Designing a wastewater treatment plant should be flexible enough to accommodate more stringent requirements, which are likely to emerge in the future. There will therefore be a continuous need for improving the reliability of current treatment methods and for exploring the feasibility of integrating several technologies: for example, (a) hybrid trickle bed reactor–reverse osmosis process for the removal of phenolic compounds from industrial wastewater effluents (Al-Obaidi et al., 2018a) and (b) hybrid photocatalytic degradation–anaerobic digestion for treating wastewater contaminated with methylene blue (Apollo et al., 2018). The combination of two and three processes in the treatment plant has already proven to offer improved contaminants removal commensurate with water quality standards. Nevertheless, the challenge of removing highly toxic compounds of very low concentrations in wastewater remains.

1.3 POLLUTANTS

According to the US Public Health Service drinking water standards, the term pollutant is a synonym of the word contaminant, which means the presence of any foreign organic, inorganic, radiological, or biological substance in water. This in turn reduces the water quality, which impairs the usefulness of the water (USPHS, 1962).

1.3.1 POLLUTANTS COMPLEXITY AND CHALLENGES

The development of resources and technologies has generated a variety of organic and non-organic chemical compounds, all of which pose a potential environmental threat (Djamel, 2018). Specifically, the increase in chemical and refinery industries over the last century contributes to the significant increase in the contamination of worldwide water systems. Even at low concentration, many micropollutants pose a greater threat when they combine to form more complex compounds. To the same extent, wastewater effluents of many industrial applications contain a variety of micropollutants, which are released into a variety of water resources. Such micropollutants not only disrupt the biological ecosystem, but they also pose a real threat to the water supply for human consumption and to aquatic ecosystems (Pomiès et al., 2013; Tizaoui et al., 2017).

Schwarzenbach et al. (2006) identified a number of complex challenges, which need to be addressed for dealing with micropollutants in water systems. They include:

- the necessity of developing special tools for assessing the impact of micropollutants on ecosystems and human health;
- the implementation of cost-effective wastewater treatment technologies;
- the control and minimisation of the disposal of critical pollutants into aquatic systems.

Even though a decade has passed since the Schwarzenbach et al. study, the challenges still exist.

Hendricks (2006) stated that thousands of contaminants may be found in wastewater. Despite the wide variety of organic compounds, this book focusses on the removal of some of the most harmful organic compounds that can be found in wastewater. Specifically, the removal of phenolic and nitrosamine compounds will be mainly addressed due to their significant relation to the wastewater treatment industry and the tighter legislation for these compounds.

1.3.2 PHENOLIC COMPOUNDS

Phenol (C_6H_5OH) and phenolic compounds are crystalline, aromatic, and colourless compounds in room temperature and are comprised of the hydroxyl and aromatic hydrocarbon groups. These compounds are mainly found as micropollutants in a wide range of concentrations in wastewater effluents of several industrial applications. For instance, they can exist in wastewater effluents of coal industry (9–6800 ppm), pharmaceutical, paint, wood products, and pulp productions (0.1–1600 ppm), petrochemical industry (28–1220 ppm), and refineries (6–500 ppm). More importantly, the phenolic compounds have a high resistance to biological decomposition due to the existence of a stable benzene ring (Ahmed et al, 2010; Mohammed et al., 2016). Chlorophenol, more persistent than phenol, is formed due to the release of phenol into the water, where it undergoes an active reaction with chlorine to form chlorophenol (Gami et al., 2014). Unfortunately, phenol and phenolic compounds are the most common harmful organic pollutants; they are carcinogenic

and can have a severe impact on human health due to their high toxicity even at very low concentrations (Busca et al., 2008; Irfanudeen et al., 2015). It is therefore not surprising to see them included in the list of toxic compounds issued by the United States Environmental Protection Agency (US EPA) (Hsieh et al., 2008). In this same respect, the European Food Standards Agency (EFSA) (EFSA, 2013) has limited the oral tolerable daily intake of phenols to less than 0.5 mg/kg of body weight/day. Jiang et al. (2003) confirmed that phenol and phenolic compounds give an intolerable taste to drinking water at about 0.5 ppm. There is therefore a strong requirement to remove the phenolic compounds from industrial effluents before discharging into surface water. Consequently, much attention has already been given by the health agencies around the world to establish tighter targets for removing these harmful pollutants from industrial effluents before disposing them into surface water. For instance, the concentration of dimethylphenol is restricted to a maximum of 0.05 ppm in surface water as recommended by the Agency of Toxic Substances and Disease Registry (ATSDR) (ASTDR, 2015). The phenol concentration in drinking water has been regulated to 0.001 ppm and to 0.0005 ppm by the World Health Organization (WHO) and the European Union (EU) respectively (Hsieh et al., 2008). The concentration of phenol in the discharge wastewater of hospitals is set to 10 ppm by the Water UK regulators (Water UK, 2011). Kamble et al. (2008) confirmed that the trace amounts of phenol and phenolic compounds in the effluents of industrial wastewater could slow down attempts to reuse wastewater in several applications.

1.3.3 N-NITROSAMINE

N-nitrosamines are organic chemicals found in reclaimed water. These by-product compounds exist at very low concentrations and are basically formed during the disinfection process of secondary-treated wastewater effluent with inhibitors such as chloramines, chlorines, and ozone (Bond et al., 2011; Brisson et al., 2013). The mechanism of N-nitrosamine formation is complicated due to the occurrences of several simultaneous reactions, which depend on the existence of inhibitors and reactant concentration (Charrois et al., 2007). However, the formation of N-nitrosamine in reclaimed water is based on two steps of reactions as follows:

1. the reaction of mono-chloramine (NH_2Cl) with unsymmetrical dimethylhydrazine (UDMH); and
2. NH_2Cl oxidises the UDMH intermediate to form NDMA (Farré et al., 2011).

The rate of NDMA formation can increase significantly when the disinfectant dose increases. However, Choi and Valentine (2002) proposed another mechanism of NDMA formation, which can be described as a reaction of chloroamines with dimethylamine during chlorine disinfection. NDMA ($\text{C}_2\text{H}_6\text{N}_2\text{O}$) (N-nitrosodimethylamine-D6) has been classified as one of the most toxic compounds in the N-nitrosamine family. This can carry severe toxicological threats to human beings. NDMA has the lowest

molecular weight of 74.05 in the N-nitrosamine family and can be found as a result of the chlorination of secondary wastewater effluent at concentrations higher than 100 ng/L (Najm and Trussell, 2001). Unfortunately, NDMA has been often investigated at higher concentrations than the legal limits in treated water supply systems including drinking water and wastewater facilities. For instance, NDMA was investigated in concentrations up to 160 ng/l in the rivers Rhine and Main in Germany (Verliefde et al., 2007). Therefore, N-nitrosamine concentration has been regulated at a very strict allowable level in drinking water and recycled water by several water authorities around the world (US EPA, 2009a). The International Agency for Research on Cancer and the US Environmental Protection Agency have classified N-nitrosamine as a potential carcinogenic compound to humans where a cancer risk level can be expected at 0.7 ng/l concentration, which is now the maximum allowed NDMA concentration in recycled water (US EPA, 2009b).

1.3.4 OTHER POLLUTANTS

Other pollutants including aniline and acrylnitrile are discussed in this section.

1.3.4.1 Aniline (Amino Benzene)

Aniline, the aromatic amine ($C_6H_5NH_2$), is common toxic persistent pollutant widely known to be carcinogenic and a harmful chemical to aquatic life (Straub et al., 1993). Aniline is an intermediate in several industrial processes, including the manufacture of pigments, rubber additives and polymers, herbicides, and pesticides, and is a solvent in perfumes, varnish, and resins (Shonall and Luthy, 1990). Aniline has solubility up to 3.5% in water and is therefore expected to be found in the industrial wastewater of these applications in addition to drinking water sources (Devulapalli and Jones, 1999). The aquatic toxicity rating for aniline is 10 ppm, and, with this concentration, it is expected to destroy 50% of any exposed organisms within 96 hours (Sánchez et al., 1998). Different treatment methods are used to remove aniline from wastewater, including adsorption (Gu et al., 2008), oxidation (Sánchez et al., 1998), distillation (Devulapalli and Jones, 1999), and reverse osmosis (Golovashin et al., 2005; Al-Obaidi-et al., 2018b).

1.3.4.2 Acrylnitrile

Acrylnitrile (C_3H_3N), a colourless volatile liquid, is a highly toxic organic compound used widely in the production of plastics, adhesives, and synthetic rubber (Bretherick, 1981). The International Agency for Research on Cancer (IARC) has included acrylnitrile as a potential carcinogenic compound (International Agency for Research on Cancer, 1999). Several treatment methods are used to remove acrylnitrile from wastewater, including biological, wet oxidation, adsorption, and membrane technology (Kumar et al., 2008). Acrylnitrile is a compound which reverse osmosis processes have struggled to remove, as confirmed by the preliminary experimental work of Bódalo-Santoyo et al. (2003) using four types of membranes. The low molecular weight of acrylnitrile is one of the main reasons of very low rejection by the reverse osmosis process (Fang and Chian, 1976).

1.3.5 HEAVY METALS

Heavy metals (known to be toxic or carcinogenic) are directly and indirectly discharged into water systems as a result of the rapid growth of chemical industries such as metal plating, mining, paper, fertiliser, batteries, and pesticides (Linnan et al., 2009; Carolin et al., 2017; Nyamayedenga, 2018). These non-degradable and high-toxic metals at low concentrations create special environmental issues due to their resistance and persistence in the environment (Peligro et al., 2016; Raval et al., 2016). They include arsenic, zinc, mercury, copper, nickel, chromium, cadmium, and lead. Chronic health issues are classified as a result of high level of exposure of these metals. For example, Oyaro et al. (2007) confirmed that a high dosage of zinc can cause severe cases of skin irritations, vomiting, nausea, and anaemia. In addition, serious lung and kidney problems are caused by exceeding the limit of nickel (Borba et al., 2006). Similarly, high levels of mercury are linked to kidney function damage (Namasivayam and Kadirvelu, 1999). Because of this, the US Environmental Protection Agency has instituted more stringent regulations for such toxic heavy metals compared to other impurities with low toxicity. For example, it has classified cadmium as a probable human carcinogen due to possibility of death at a high level of exposure (Huff et al., 2007). Fu and Wang (2011) reviewed the most efficient methods used to remove hazardous heavy metal from wastewater, which include ion exchange, adsorption, and membrane technology. They concluded that ion exchange, adsorption, and membrane filtration and especially RO process are the most effective and economical methods commonly used to remove heavy metals from wastewater. Generally, pretreatment methods, including the precipitation method, has always been used as a favoured method for removing heavy metals. However, one of main concerns of non-degradable heavy metals is their disposal into surface water as they convert to hydrated ions, leading to higher level of toxicity compared to the original metal atoms. Additionally, when heavy metals are combined, their removal from water can be even more challenging (Carolin et al., 2017).

1.4 CONCLUSIONS

This chapter has briefly outlined one of the biggest challenges of the world today, which is water. It has highlighted key environmental problems associated with the discharge of after-use water, i.e. wastewater from different types of applications (domestic, agriculture, industrial) into the water sources and the challenges associated with it. This chapter has also discussed highly toxic organic compounds from such discharges. The awareness created by several health agencies in respect to these toxic compounds is also highlighted. The chapter has emphasised the urgent need for efficient and cost-effective wastewater treatment methods and technologies together with analytical techniques required for removing harmful contaminants at low concentrations.

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2 Wastewater Treatment Methods

2.1 INTRODUCTION

Modern industrial facilities combining several types of technologies have introduced a variety of highly toxic chemicals (contaminants) in industrial wastewater. These have significantly increased the level of potential environmental harm to humans, animals, and the ecosystem. Several attempts have been made to overcome the challenges of removing such contaminants from wastewater including many technologies and analytical techniques for detecting these contaminants, even in low concentration. However, many such attempts have limited success in completely removing complex by-products such as N-nitrosamine (Petrovic et al., 2003; Fujioka et al., 2018).

Much attention has already been paid to establishing tight targets for removing these harmful contaminants from industrial effluents before discharging then into the water cycle. A number of precautionary measures have therefore been used to monitor their release. For example, the European Community on Risk Assessment and Directive has made an important amendment on the cataloguing of dangerous compounds (European Commission, 2011), which now includes such harmful compounds. The European Union documented only 66 chemicals in 2000 as being endocrine-disrupting chemicals (EDCs), including pharmaceuticals, surfactants, personal care products, industrial additives, and a variety of numerous chemicals. However, the priority list has significantly increased to 564 chemicals in 2009 (Bolong et al., 2009). The presence of emerging toxic compounds in wastewater has become a major worry due to their passive impact on all living organisms. The pollution of water resources systems (rivers, oceans, and groundwater) is a direct result of significant recycling of a variety of wastewater, including sewage, untreated industrial wastewater, landfill, and agricultural pathway wastes. Since reclaimed wastewater has become one of the most tangible solutions for global water scarcity, the development of more effective technologies for wastewater treatment has become a priority in many countries. To this extent, there has been a noticeable increase in innovative and diverse water treatment technologies due to strict water quality regulations with emphasis on trace contaminants (Abdulgader et al., 2013).

Whilst the book focusses on applications of the reverse osmosis (RO) process as a promising technique for the removal of organic compounds from wastewater (reusing and reclaiming wastewater), this chapter presents a detailed review of the most efficient and advanced treatment methods for removing organic pollutants from wastewater.

2.2 OVERVIEW OF WASTEWATER TREATMENT METHODS

Wastewater treatment methods are complex processes compared to standard drinking water treatment methods due to the existence of several types of contaminants. Wastewater effluents require an extensive treatment before safely releasing them to the environment. Several wastewater treatment methods capable of treating industrial effluents are available. Each treatment method has advantages and disadvantages. The successful wastewater treatment method is the one that can reduce dependence on freshwater (water conservation) by efficiently and sustainably recycling wastewater (reuse water) for industrial use at low energy consumption. Several parameters to consider include the nature, organic concentration, and complexity of pollutants in the wastewater, which determine the performance of given technologies used (Santos et al., 2005). This section outlines wastewater treatment technologies used to remove micropollutants from wastewater (Jain et al., 2004; Lee et al., 2005; Busca et al., 2008; Bolong et al., 2009; Abdulgader et al., 2013; Mohammed et al., 2016). They include:

1. Physicochemical treatment methods: These include the coagulation–flocculation process and adsorption by activated carbon, especially for diluted aqueous solutions.
2. Biological treatment methods: These methods are usually denoted as sewage treatment methods, which include activated sludge and biological trickling filters. Specifically, these methods use clarifiers to renovate the organic micropollutants into an easily separated biomass.
3. Advanced treatment methods: These methods comprise a variety of highly efficient methods embedding the microbiological safety of the reclaimed water. They include:
 - Ultraviolet (UV) photolysis.
 - Ion exchange.
 - Electrochemical oxidation (chlorine and hypochlorite).
 - Photo oxidation processes where phenol oxidation activity is under UV irradiation.
 - Oxidation with chemical oxidants (O_3 ozonation and H_2O_2).
 - Membrane bioreactor process.
 - Oxidation with air processes, including non-catalyst and catalyst wet air oxidation.
 - Specifically, the oxidation method using chlorine or ozone are classified as a highly graded treatment technology.
4. Membrane filtration technology such as nanofiltration and reverse osmosis (RO) treatment methods.
5. Hybrid systems, such as:
 - Membrane bioreactor: A combination of the activated sludge process with micro- or ultra-filtration membrane separation.
 - Photocatalysis, which is integrated with a membrane: The membrane can be used as a barrier for the photocatalyst and a selective barrier for the pollutants to be removed. Photo degradation of organic compounds from wastewaters is used with TiO_2 as a photocatalyst.

Most recently, a number of the aforementioned treatment methods and a few alternative methods have been applied to remove specific contaminants from wastewater. Mujtaba et al. (2018) explored a number of such wastewater treatment processes.

Amosa et al. (2018) studied pore-blocking behaviours of low-pressure membranes for wastewater treatment while Mathaba and Daramola (2018) used composite membrane materials for metal removal from wastewater. Al-Obaidi et al. (2018a, 2018b) used an RO process for the removal of phenolic compounds and eight selected organic and inorganic compounds from wastewater. Waterborne pathogens in municipal water were inactivated by using ozone (Mecha et al., 2018). Synthetic dyes are extensively used in many industries and the azo dyes correspond to more than 60% of manufactured synthetic dyes. Methylene blue (MB) is the most commonly used azo dye in paper and in textile industries and contributes to the generation of wastewater. Biosorption of methylene blue dye from wastewater using anise tea residue was explored by Hassan et al. (2018).

2.2.1 PHYSICOCHEMICAL TREATMENT METHODS

Some of the effective wastewater treatment methods are highlighted in this section.

2.2.1.1 Coagulation and Flocculation

The term coagulation refers to the reaction between selected chemical and colloidal particles (suspension molecule has a density equal to water density) to form a microfloc. The coagulation treatment process is mainly used in wastewater treatment to remove various particles including clays, natural organic matter such as humic acids (HA), and microscopic organisms of viruses, algae, and bacteria found commonly in water (Dobias and Stechemesser, 2005; Ersoy et al., 2009). In respect of heavy metal removal from wastewater, coagulation is used to precipitate metals to form low soluble compounds such as carbonates, hydroxides, and sulphides (Visa, 2016). The conventional chemicals used in coagulation are generally alum Al^{+3} or a ferric salt Fe^{+3} that form hydrolysis compounds, which react with negative charged particles to form a microfloc. The microflocs are then combined due to collisions, and polymeric materials are used as an aid for flocculation (known as flocculant) to create bonding between floc particles to form larger particles which can settle down easily. The effectiveness of coagulation treatment is based on the right selection of coagulant (type), dosage along with pH, alkalinity, temperature, and mixing conditions, which includes turbulence intensity, circulation pattern, and residence time (Environmental Protection Agency, 2002; Renault et al., 2009; Ghernaout et al., 2011; Bratby, 2016). The coagulation and settling step is followed by filtration processes to remove any remaining suspended particles in the wastewater. Several experimental works can be found in the literature on the use of metal coagulant such as aluminium sulphate for the removal of inorganic contaminants from activated sludge secondary effluent. Several types of coagulants of aluminium and ferric compounds were used by Fan et al. (2003) to remove arsenate from wastewater. The order of removal efficiency is found to be as aluminium sulphate > aluminium chloride > polyaluminium sulphate > polyaluminium chloride. Specifically, the experiments confirmed the best removal is between 41% to 89% at dosages of 0.8 to 1.9 mg/l of aluminium and pH

of 5.5. This is true for amalgamation of coagulation and sedimentation at an initial arsenic concentration of 50 $\mu\text{g/l}$. However, the removal can be increased from 59% to 99% with the addition of filtration after sedimentation. In particular, the efficiency of removing inorganic compounds from wastewater is originally based on the contaminant itself and oxidation state. More particularly, the rate of adsorption of the contaminant onto particulates can determine the extent of its removal. Westerhoff et al. (2005) conducted a study in a bench-scale water treatment plant and tested the removal of several endocrine-disrupting chemicals as well as pharmaceuticals and personal care products from three surface waters and a synthetic model water containing 10 ng/l of any specific compound. The results confirmed that physico-chemical treatment by aluminium sulphate and ferric chloride coagulants are not effective for removing EDCs, pharmaceuticals, or personal care products. Moreover, the removal of these compounds was independent of the initial compound concentration in the wastewater.

El Samrani et al. (2008) used ferric chloride solution and poly-aluminium chloride to degrade the existence of heavy metal in a combined sewer overflow (domestic sewage). This confirmed an efficient turbidity removal (efficient clarification) with both coagulants at lower optimum dosage. Interestingly, optimum turbidity removal attained an outstanding removal rate of heavy metals based on optimum concentrations. However, one of the main imperfections of the coagulation treatment method is the sludge formation (by-products like flocks), which occurs as a result of the aggressive usage of chemicals (Carolin et al., 2017). This may often add new pollutants to the passive impact of chemical solvents on the environment.

2.2.1.2 Activated Carbon Adsorption Method

Activated carbon adsorption (ACA) is used in several industries, including drinking water treatment and advanced industrial wastewater treatment for removing organic pollutants in line with rigorous regulations before discharging wastewater into surface water. Specifically, ACA includes the removal of substances which affect odour and taste and relates to a wide range of organic compounds such as herbicides, pesticides, phenols, acids, high molecular weight aliphatics and amines, esters, etc. (Hendricks, 2006). The effectiveness of the adsorption method is measured in terms of the extent to which the targeted pollutant concentration is reduced in the treated water. The ACA process was originally used as a separate process or connected to filtration and coagulation processes in industrial facilities. It can be considered as a pretreatment step to a biological treatment, which mitigates toxic compounds from wastewater (Ye, 2016). Several examples in the open literature confirm the effectiveness of activated carbon adsorption to remove micropollutants from wastewater. For instance, Selvi et al. (2001) used batch mode adsorption of activated carbon for the removal of hexavalent chromium Cr (VI) (more highly toxic than other valences) from aqueous solution with particle size ranged between 125 and 250 μm . The experiments were carried out at different chromium and carbon initial concentrations, agitation times, and pHs. This in turn showed the feasibility of acidic medium for the efficient removal. Also, two powdered activated carbon brands were tested by Westerhoff et al. (2005) and confirmed the removal of almost 90% of endocrine-disrupting chemicals. However, some other compounds are only removed

within a 40%–60% range. The removal efficiency is dependent on the initial concentration, contact time, and activated carbon dosage. However, the effectiveness of ACA is limited when used for removing low molecular weight and high polarity compounds such as N-nitrosamine and glycols (Groeber, 1991). Beker et al. (2010) tested the removal of phenol from an aqueous solution using a patch adsorption process of cherry stone-based commercial activated carbon (agricultural by-product) type Chemviron CPG-LF and two polymeric adsorbents (MN-200 and XAD-2). The experiments were carried out at 25 mg/L 30 °C of initial phenol concentration and temperature with a medium of 6.5–9 pH solution. This yielded a phenol removal of around 90% by activated carbon compared to other polymeric adsorbents. Most recently, El-Tahhan (2018) used activated charcoal and treated rice husk (TRH) to remove chromium ions from wastewaters using adsorption techniques.

2.2.2 BIOLOGICAL TREATMENT METHODS

The biological treatment method constitutes the use of microbes to remove natural organic compounds from wastewater. Activated sludge process (ASP) and membrane bioreactors (MBRs) are the most generally applied biological wastewater treatment methods. These are progressively used in many industrial applications, such as landfill and conventional municipal wastewater treatment. In essence, a membrane bioreactor is a modified version of ASP, in which a membrane separator is used instead of a secondary clarifier of ASP (Jiang et al., 2009). The removal of micropollutants includes a wide range of emerging contaminants such as volatile organic compounds, pesticides, surfactants and hormones, and pharmaceutical substances. It is carried out in the activated sludge systems by a bacterial biomass suspension in three steps: volatilisation to air, sorption to the sludge, and biological conversion (Gernaey et al., 2004; Pomiès et al., 2013). Most importantly, as the removal of nutrients (ammonia nitrogen) from wastewater is becoming a priority and there is stringent regulation to limit its discharge into surface water and groundwater, the activated sludge and membrane bioreactor wastewater treatments are progressively used to remove nitrogen and biological phosphorus in addition to organic compounds (Ahn et al., 2007). Specifically, the sludge and biological trickling filters can alter aqueous organic compounds into biomass that can settle easily. In this context, several studies confirm the suitability of MBR over ASP for removing nutrients efficiently (Adam et al., 2002; Phagoo et al., 2005; Daigger et al., 2005; Monti et al., 2007).

A considerable amount of research in the literature is directed to test the efficiency of ASP and MBR processes that have been applied in several types of wastewater. Most studies exhibit a promising degree of organic and nitrogen removal with a few limitations, and some examples illustrating this are discussed in the following section.

Visvanathan et al. (2007) tested the performance of a thermophilic membrane bioreactor to treat raw landfill leachate from two landfill sites in Thailand. The examined feed properties were within the ratio of biochemical oxygen demand (BOD) to chemical oxygen demand (COD) of 0.39, 0.57, and 0.65. It was found that MBR could reduce 97%–99% and 62%–79% of BOD and COD, respectively. However,

the increase in BOD and COD reduction led to a decrease of ammonia removal from 75% to 60% with an increase in a BOD/COD ratio of the feed.

Ahn et al. (2007) used the combination of upflow sludge bed filter (anaerobic) and aerobic MBR to treat a high concentration of nitrogen in wastewater. The average removal efficiencies of organics and nitrogen were found to be 99% and 46%, respectively. However, the observed operation of the combined process of bed filter and MBR required nine times the transmembrane pressure (TMP) than that of an individual MBR unit working under the same operating conditions. Severe fouling impact of the combined process causes this increase of TMP due to increased extra-cellular polymeric substance and hydrophobicity.

Zuthi et al. (2012) reviewed the efficiency of biological treatment methods of ASP and MBR to remove phosphorus from wastewater and found that the performance of ASP and MBR was mainly dependent on several parameters, including sludge and hydraulic retention times, temperature, organic loads, alkalinity, and pH.

Some limitations of the use of ASP and MBR (biological treatment methods) are highlighted below:

- These methods are not effective for removing inorganic pollutants such as heavy metals¹ (toxic even at low concentration) from wastewater. This is due to their specific characteristics of solubility, oxidation, and complex formation. Heavy metals are not easy to decompose, which complicates the treatment process (Lee and Pandey, 2012).
- Formation of sludge as by-products (Ozaki, 2004; Urase and Kikuta, 2005).
- Some compounds are exempted from completely converting to biomass, such as the estrogenic alkylphenols and steroid estrogens found in effluents (Johnson and Sumpter, 2001).
- Biological trickling filter case is not able to remove estrogens due to their low sludge retention time and hydraulic retention time (Servos et al., 2005).
- The fouling and permeability loss of membrane bioreactors caused by the accumulation of macromolecular components of the activated sludge at the membrane surface leads to the formation of a cake layer of colloidal fouling, which significantly reduces the driving force (Wintgens et al., 2003). Therefore, the fouling is considered as one of the imperfections of this process, which retards the flux performance. To rectify this concern, chemical cleaning using cleaning agents and permeate back flushing are extensively used, with realising the possibility of membrane damage (Kornboonraksa et al., 2009).

Interestingly, the amalgamation of activated sludge units and membrane filtration for biomass retention cause a high removal of impurities (Wintgens et al., 2003).

2.2.3 ADVANCED TREATMENT METHODS

Advanced treatment methods include several options for removing micropollutants from wastewater, such as ultraviolet (UV), chlorination, ozonation, and photolysis. The next sections highlight some examples of these treatment methods.

2.2.3.1 Advanced Oxidation Process

Advanced oxidation processes are commonly used as a highly viable water treatment method for the removal of stable chemicals and low biodegradable organic pollutants due to the high oxidation potential of active oxygen species. In this respect, the dissolved organic carbon (DOC) concentration and the chemical oxygen demand (COD) are the two indicators widely used to describe chemical oxidation (Scott and Ollis, 1997; Oller et al., 2011). Simply put, the oxidation process means the transformation of a compound from one species to another using an oxidising agent. As natural organic compounds become an issue, the oxidation process is an alternative solution to degrade hazardous compounds in wastewater in addition to dealing with taste and odour (Rasalingam et al., 2014). It is important to note that biological treatment processes are not efficient for dealing with taste and odour. The main oxidative agents used are ozone, chlorine dioxide, and potassium permanganate (KMnO_4). The use of these oxidants has progressively evolved in several countries in a variety of wastewater treatment applications. However, Germany has the larger number of municipal wastewater treatment facilities which use ozone to deal with taste and odour. The use of ozone as an oxidising agent started in 1996 in drinking water industries (Kaminski and Prendiville, 1996). Chlorine dioxide and potassium permanganate were used in drinking water treatment half a century ago (Babbitt and Doland, 1949). However, the use of chlorine dioxide as a disinfection and as a useful oxidant to degrade Mn^{+2} or Fe^{+3} in domestic wastewater treatment is noticeably reduced due to the formation of trihalomethanes (by-products) (Jones, 2009). Also, the formation of rusting in the oxidation treatment process is noticed due to the use of such oxidants.

Chlorine and ozone are strong oxidisers having high reactivity against organic compounds, especially at low dissolved organic compounds. The literature contains several studies of advanced oxidation processes, and some examples of these are illustrated in the next section.

Westerhoff et al. (2005) showed that chlorination and ozonation treatments could remove less than 90% of aromatic rings of pharmaceuticals compounds with an excess removal of 5%–15% after addition of hydrogen peroxide H_2O_2 prior to ozonation compared to ozone alone. However, the chlorination and ozonation treatments may produce by-products of unknown impacts that require extra precautions. This is already consistent with the findings of Suffet et al. (1995), Szewzyk et al. (2000), Zhang and DiGiano (2002), Petrovic et al. (2003a), Sadiq and Rodriguez (2004), Vieno et al. (2006), and Gopal et al. (2007).

Huber et al. (2005) tested the ozonation treatment in a pilot-scale plant consisting of two bubble columns to release pharmaceuticals and endocrine disruptors of various concentrations of suspended solids from the effluents of three wastewater treatment applications. Several pharmaceuticals were oxidised by more than 90%–99% for O_3 doses of more than 2 mg/l in all effluents. Also, it was noticed that the total suspended solids present in wastewater had insignificant impact on the oxidation efficiency where 5 mg/l was required for high concentrations of suspended solids.

Lan et al. (2008) proved the efficacy of ozonation process in the mineralisation of a complex mixture of the relatively low organic compounds present in cork-processing water. The ozonation experiments were carried out in a bubble column

semi-batch reactor using a varied flow rate of ozone/oxygen mixture. It was found that a more than 90% reduction in total organic carbon (TOC) and chemical oxygen demand could be achieved in the deep mineralisation of organic matter. This is comparable to the reported results of Silva et al. (2004), who showed a low performance of photo oxidation processes involving TiO_2 photocatalysis and hydrogen peroxide to mineralise organic pollutants.

Lucas et al. (2009) studied the performance of a pilot-scale bubble column ozonation reactor to degrade organic substances present in winery wastewater, which showed significant degradation of aromatic and polyphenol substances in the wastewater.

2.2.3.1.1 Catalytic Wet Air Oxidation (CWAO) Process

The process of catalytic wet air oxidation, or CWAO, is a well-known wastewater treatment method and one that is gradually becoming prevalent in the treatment of various industrial toxic and refractory wastes. Typically, the process oxidises the organic compounds in aqueous phase using normal air or pure oxygen inside a trickle bed reactor (TBR) packed with solid catalyst (Figure 2.1). The oxidation

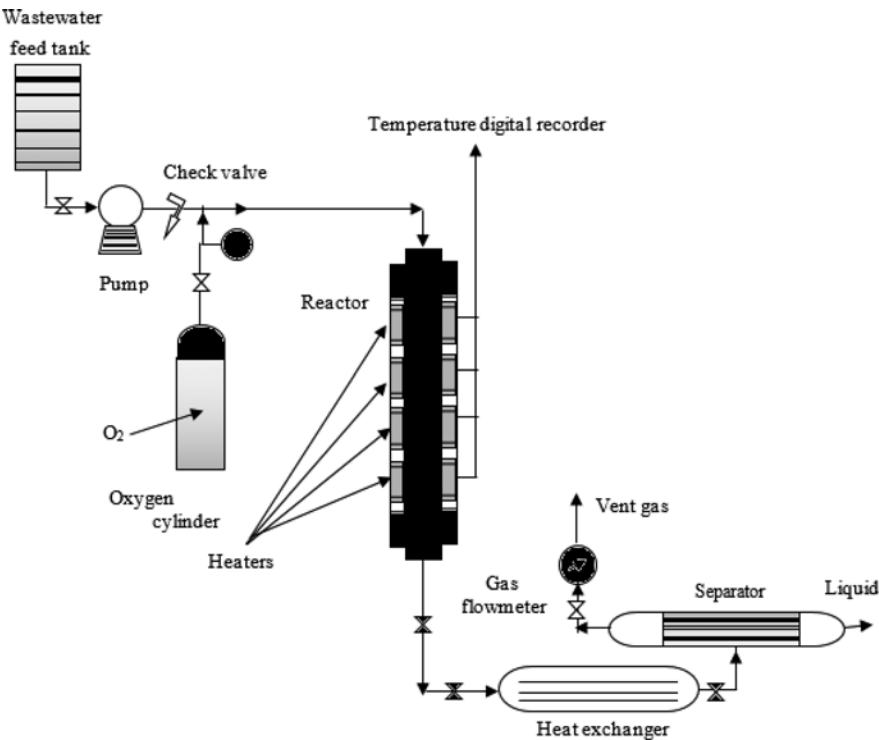


FIGURE 2.1 Schematic diagram of the CWAO process.

(Adapted from Mujtaba et al., 2018)

of organic matter is carried out at a specified range of the operating conditions of the reactor between 100 and 350 °C and 4.93 to 197.38 atm of reaction temperature, and pressure, respectively (Safaa, 2009; Mohammed et al., 2016). The other operating conditions include initial organic compound content, oxygen partial pressure, wastewater hourly space velocity, and gas flow rate. The treatment process includes a heat exchanger to monitor the temperature of the hot outlet reactor stream, besides the existence of a separator to separate any remaining gas (Mohammed et al., 2016). As the process operates at higher pressures and temperatures requiring high energy input, a significant amount of energy can be recovered and reused within the system by appropriately designing a heat exchanger network for the process (Mohammed et al., 2017). Mohammed et al. (2016) confirmed that CWAO could remove between 60% to 90% of phenol from wastewater based on the operating conditions.

2.2.3.2 Limitations of Conventional Treatment Methods

Several detailed reviews were carried out by Fu and Wang (2011), Amin et al. (2014), Patil et al. (2016), Carolin et al., 2017, Azimi et al. (2017), and Krishnan et al. (2017) regarding the deployment of a number of traditional treatment methods for the removal of toxic heavy metals from wastewater. These studies highlighted the following limitations of these methods:

- One of the concerns with the activated sludge process (biological treatment method) is the deficiency of dealing with several emerging contaminants where these compounds remain soluble in the wastewater after the treatment.
- Inefficiency of coagulation, flocculation, and lime softening methods (physicochemical treatments) to remove several pharmaceutical and EDCs has been observed.
- Several disinfection by-products and unwelcome tastes and odours are induced by the chlorination treatment method (oxidation process), despite it providing a protection against several types of pathogens and bacteria.
- The oxidation method using ozone can be very expensive.
- Ultraviolet (UV) photolysis and ion exchange are not suitable for the effective mitigation of some micropollutants (Adams et al., 2002).

2.2.4 MEMBRANE TECHNOLOGY TREATMENT

Membrane technology comprises microfiltration (MF), ultrafiltration (UF), reverse osmosis (RO), and followed by nanofiltration (NF) processes, which are effective pressure-driven filtration processes (Van der Bruggen and Vandecasteele, 2002; Qin et al., 2007; Walha et al., 2007; Al-Obaidi et al., 2018, 2018a, 2018b). Membrane technology treatment was initially developed for the desalination of seawater and brackish water to produce drinking water (Sassi an Mujaba, 2013; Al-Obaidi et al., 2018c). However, its rapid growth in various applications has rendered this technology a commercially attractive separation process for the treatment of industrial effluents. The technology has been used for removing several

organic micropollutants from wastewater (Kiso et al., 2001; Bodzek et al., 2004; Yoon et al., 2006; Srinivasan et al., 2010; Fujioka et al., 2013; Al-Obaidi et al., 2018, 2018a, 2018b) and is now recognised as a promising technology for wastewater treatment. Specifically, the RO process yields low levels of pollutant concentration in the permeate, which in turn accelerates the reclamation of good-quality water for yet more applications (Al-Obaidi et al., 2018, 2018a, 2018b). However, the RO process consumes higher energy when compared to the NF process (Braeken et al., 2006). The performance of membrane technology is based on several parameters, including feed concentration, operating pressure, particle size, and pH (Barakat and Schmidt, 2010). The membrane permeability relies on the pore size of the membrane material (Fu and Wang, 2011). The mechanism of transportation and pollutants removal is summarised by three mechanisms of convection, diffusion, and charge effect (Braeken et al., 2006). In this respect, the transmembrane pressure drives the convection while the concentration difference across the membrane sides causes the diffusion mechanism. However, the membrane pore size and target compound size play an important role in the diffusion mechanism through the membrane surface. Therefore, any compound of molecular size larger than membrane pore size would not be able to penetrate through the membrane due to the sieving impact of membrane structure (Verliefde et al., 2007). Lastly, the electrostatic repulsion between the charged organic matters and uncharged membrane surface leads to the third mechanism. Specifically, the ionic and low molecular weight compounds are rejected by membranes due to charge repulsion (Hilal et al., 2004). Undoubtedly, the above mechanisms control the separation performance of organic compounds in line with the pollutant type. Kimura et al. (2003) used a bench-scale filtration system of thin-film composite NF and RO membranes for the removal of organic micropollutants such as disinfection by-products (DBPs), endocrine-disrupting chemicals, and active pharmaceutical compounds (PhACs). The study showed a high removal of negatively charged organic compounds of up to 90% due to the electrostatic repulsion mechanism with a negatively charged membrane surface of carboxylic acid or sulphonic groups. However, the pore size of compound affected the rejection of uncharged organic compounds due to the sieving mechanism. It was also observed that high feed concentration of $\mu\text{g/L}$ led to higher removal of organic compound compared to low feed concentration of ng/L . The rejection of RO membrane was found to be higher than that by NF membrane.

Tang and Chen (2000) examined the performance of the crossflow of thin-film composite polysulphone NF membranes to treat strong-coloured synthetic textile wastewater with highly concentrated inorganic dissolved salts. They observed high flux at low pressure of 4.93 atm while 98% of the dye was removed. However, low rejection of NaCl was reported at around 14%. This shows the importance of operating conditions such as dye concentration, operating pressure, crossflow velocity and electrolyte concentration to drive the rejection of contaminants.

Verliefde et al. (2007) reviewed and assessed the performance of NF membranes for the removal of persistent organic micropollutants in the Dutch and Flemish water sources. The qualitative prediction of NF and RO membrane rejection performance was conducted based on several indicators of key solute and membrane parameters in the nanofiltration process. These indicators included:

- The acidity constant pK_a of the solute (solute charge indicator) linked to the feed pH. Therefore, it can be said that negatively charged organic compounds are more rejected due to negatively charged NF membranes.
- The polarity defining the electrostatics interaction with the membrane charge and hydrophobicity, where hydrophobic interactions increase the accumulation of solutes on the membrane surface and its adsorption into membrane pores. The parameter octanol-water partitioning coefficient ($\log K_{ow}$) was used to express the hydrophobicity. The higher $\log K_{ow}$ meant higher adsorption to the membrane and easy permeation through the membrane pores.
- The molecular size of the solute, which plays an important role to solute rejection based on a size exclusion basis.
- The hydrophilic compounds are soluble in water. However, the coalition of the hydrophilic molecule with water molecules might cause a bigger effective diameter of the molecule that results in a higher rejection.

It is noteworthy to mention that the previously mentioned indicators can be used to predict the performance of NF membranes against the removal of highly toxic compounds.

The impact of operating parameters such as pressure, temperature, and concentration on the rejection parameter of wastewater treatment is related to the targeted compounds and membrane characteristics. For instance, increasing the operating pressure leads to higher water recovery and rejection, whereas high operating pressures may lead to rejection parameter reduction (Verliefde et al., 2007). More details on the impact of operating conditions will be discussed in Chapter 7.

Membrane technology is a much cheaper treatment method than conventional treatment processes. It has many advantages, including ease of operation, readiness to be scaled up, less space requirement, minimum thermal damage, and lower energy consumption compared to conventional treatment methods (Fu and Wang, 2011; Reverberi et al., 2014). However, a major problem of membrane technology (especially NF and RO processes) is the fouling and periodic replacement of membrane. Fouling can be degraded by using pretreatment methods that can enhance the process performance for a long time of operation (Tran et al., 2015). Having said this, the removal of highly toxicological compounds from wastewater remains a challenge with membrane technology. Fu and Wang (2011) reviewed and assessed several treatment techniques which have been used to remove heavy metals from wastewater. This study affirmed that the ion exchange process has been commonly used to eliminate metals from wastewater. Similarly, the use of low-cost adsorbents has been found to provide an effective and economic treatment method. However, this is only true for low concentrations of heavy metals in wastewater. Interestingly, good results for removing heavy metals from wastewater have been achieved using membrane technology (Patil et al., 2016), and this has encouraged membrane manufacturers to improve the texture of the membrane.

In summary, Table 2.1 gives an overview of the specific characteristics of each wastewater treatment technology, its performance for the removal of organic and highly toxic compounds from wastewater, and its limitations.

TABLE 2.1
Summary of Advantages and Disadvantages of Wastewater Treatment Methods

No.	Wastewater treatment method	Advantages	Disadvantages
1	Coagulation and flocculation	Low-cost process	Sludge formation Use of several chemicals
2	Adsorption	Easy operation Less sludge production Economic treatment method	Not efficient for high-concentration heavy metal
3	Biological treatment	Effective for organic and nitrogen removal	Sludge formation Cannot deal with several emerging contaminants
4	Advanced oxidation	No need of electricity	Rusting problems High cost of ozone Produces by-products Unwelcome tastes and odours
5	Membrane system	Easy operation Lower space requirement Easy to be scaled up Minimum thermal damage Efficient to remove heavy metals Energy requirements are low	Membrane fouling Periodic replacement Limited removal of high toxicological compounds Delicacy of the membranes

2.2.5 HYBRID SYSTEMS

Hybrid systems are essentially configurations consisting of two or more of the conventional processes for enhancing the rejection of contaminants. These have been found to be significantly better than those achieved by individual conventional processes. Their combined use can help overcome weaknesses of individual treatment processes. For example, biological processes, such as the activated sludge process, cannot treat wastewater with dyes due to the high concentration of heavy metals such as chromium and lead that are toxic to microbes (Dionisi, 2014; Azimi et al., 2017). Also, the contaminant level in the treated wastewater from an individual treatment method may not comply with regulatory effluent discharge requirements (Sapari, 1996) and may require further treatment. A secondary treatment may therefore be required. To address this, several examples of hybrid processes have been proposed for wastewater treatment resulting in enhanced quality of water, reduced cost of production, energy savings, and environmental compliance (Ang et al., 2015; Altaee and Hilal, 2015). Lin and Chen (1997) tested a combination of electrochemical method, chemical coagulation, and ion exchange to treat and reuse secondary wastewater effluent of a dyeing and finishing mill. These methods are effective for removing colour, turbidity (NTU), COD concentration, Fe, and total hardness of the

wastewater. However, the total dissolved salts (TDS) cannot be removed effectively, which underscores the importance of combining this with an RO process. It seems that the use of an RO process is critical for completely removing organic matters from wastewater.

Unquestionably, the wastewater treatment technology is entirely dependent on the quality of reclaimed water. To this extent, media filtration can be used as a secondary treatment method after the wastewater treatment to be used for irrigation or cooling tower waters. However, the combination of several treatment methods of microfiltration, RO, and oxidation technology is required for guaranteeing high-quality reclaimed water (Wade Miller, 2006). Geraldles et al. (2008) used a combination of coagulation/flocculation steps and a dissolved air flotation (DAF) step as a pretreatment process for a spiral wound module nanofiltration to eliminate colloidal matter and suspended solids from Tagus River surface water (Valadas, Portugal). The output of this hybrid process showed a modification of both the silt density index (SDI)² and the fouling index of the treated water, which are always used to estimate the concentration of pollutants. Moreover, a hybrid system combines the membrane flotation process (air diffusers) and commercial spiral wound RO and NF membrane modules proposed by Soudilovski et al. (2008) for the removal of copper and other heavy metals from wastewater. This showed a high removal of harmful pollutants and with high water recovery. Al-Zoubi et al. (2009) developed a hybrid DAF–membrane process for the treatment of several types of wastewater. Furthermore, Kim et al. (2009) combined granular activated carbon (GAC) and MF membrane in a hybrid system for water purification and wastewater reclamation/reuse. The selected performance indicators included the dissolved organic carbon (water quality) and permeate flux (water quantity). This study affirmed the effectiveness of the hybrid process in wastewater treatment compared to the individual MF membrane process.

Kornboonraksa et al. (2009) investigated the hybrid process of the chemical precipitation (CP) and membrane bioreactors (MBRs) for the treatment of piggery wastewater. Generally, piggery wastewater holds a high amount of stable colloids of nitrogen, phosphorus, and high amounts of organic matters. The chemical precipitation is an efficient method to remove solids. However, soluble organic substances and nutrients are not effectively removed. Therefore, the presence of MBRs as a secondary treatment step is usually used to abate the soluble organic compounds. The adopted hybrid process has proved to be highly efficient for organic oxidation and nitrogen removal. Statistically, 99.5%, 99.4%, 99.8%, and 98.2% of BOD, COD, turbidity, and $\text{NH}_3\text{-N}$, respectively, were removed by the chemical precipitation and MBR hybrid process.

Mozia et al. (2016) have experimentally assessed the integrated system of the bed biofilm reactor (HMBBR), UV/O₃ advanced oxidation (photoreactor), UF and NF membrane steps for treating and reusing industrial laundry wastewater. This study confirmed the high removal rates of organic pollutants of the laundry wastewater. Pimple et al. (2016) proposed an integrated system for removing highly toxic pollutants of cyanides and phenols from the coke-oven wastewater. In this respect, the hybrid system comprises UF, membrane bioreactor, and RO processes, which ultimately produces an effluent that can be used for recirculation and horticultural practices. The integrated system achieved a rejection of $90 \pm 2\%$ and $95 \pm 3\%$ of cyanides and phenols, respectively.

The success of the aforementioned hybrid technologies in wastewater treatment can therefore be attributed to the use of individual methodologies in a combinative and supporting manner. Experimental results of many such methodologies when used in isolation, such as pilot-scale TBR and RO processes, have confirmed that they do not achieve the required high phenol rejection rate (Al-Obaidi et al., 2018).

To sum up, it can be said that wastewater treatment methods are core technologies for producing reclaimed and reused water, which is suitable for use in many industrial applications. Combined methods such as those discussed in this chapter will contribute to providing potential sustainable solutions for tackling the increasing demand for water.

2.3 CONCLUSIONS

The demand for high-quality water is progressively increasing around the globe as a result of the growing population, which requires sustainable food, energy, and water. More specifically, the modern industrialised world will continue to demand even larger amounts of water required in all aspects of life, but would also produce vast amounts of harmful wastewater. There is no doubt that the treatment of wastewater for reuse will become the number one priority for many countries despite cultural and social barriers (Mujtaba, 2012; Mujtaba et al., 2018a, 2018b; Mujtaba, 2019a, 2019b). This will provide a stronger motivation for the development of innovative treatment methods for removing micropollutants from wastewater and providing water of suitable quality for reuse in domestic, agriculture, and industrial applications. Pollutants found in wastewater have direct and indirect potential impacts on human health. Unquestionably, organic and highly toxic compounds have become one of the most serious environmental issues due to their persistent occurrence in many different types of wastewater.

This chapter has reviewed and evaluated various technologies used for removing pollutants and highly toxic organic compounds from wastewater. Conventional treatment technologies have yielded a relatively acceptable rate of abating a good number of organic compounds. However, they do not cope well with several other highly toxic organic compounds, which can easily pass through the treatment method due to their size (usually in micro- or nanograms/litre). This is where the use of membrane technology can provide a better and cheaper removal rate of such organic compounds. To this extent, the following observations can be made:

- The low-concentration endocrine-disrupting chemicals continue to pose a threat to the water supply network (Tizaoui et al. (2017).
- Each individual treatment technology has its own restrictions and limitations, but well-designed combinations of several technologies can address the limitations of individual processes.
- The continuously increasing demand for reused water will increase the challenge of identifying and using the most effective treatment method with the lowest energy consumption.
- Interest in membrane technology used in wastewater treatment is growing rapidly. The development of effective membrane structures with low/

no fouling need to be explored to guarantee the elimination of unregulated chemicals (Galiano et al., 2018).

- The efficient removal of contaminants in membrane technology is based on the specific properties of the targeted compound, size, and charge exclusions.
- The removal of small polar organic compounds and newly emerging micro-pollutants such as NDMA (N-nitrosodimethylamine) and MTBE (methyl tertiary-butyl ether) continues to be a challenge despite several attempts, and further research is required.
- The integration of the chemical precipitation activated carbon adsorption, ozonation, and membrane technology as a hybrid process can provide effective solutions, which will comply with the limits of organic compounds in wastewater effluents.

NOTES

- 1 Heavy metal has an atomic weight between 63.5 and 200.6 and a specific gravity more than 5.0 (Srivastava and Majumder, 2008).
- 2 The silt density index is a measure for the fouling capacity of water in reverse osmosis systems. The test measures the rate at which a 0.45-micrometre filter is plugged when subjected to a constant water pressure of 206.8 kPa (30 psi). The SDI gives the percent drop per minute in the flow rate of the water through the filter, averaged over a period such as 15 minutes (Water Treatment Guide).

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3 Membrane Processes

3.1 INTRODUCTION

The need to treat and reuse water has never been greater in the modern world we live in. Membrane technology has undoubtedly affirmed its suitability and effectiveness for removing a wide range of impurities at lower specific energy consumption compared with traditional wastewater treatment processes. In this respect, there has been considerable progress in the past decade to improve the performance of separation processes, including more specifically reverse osmosis (RO) membrane purification systems. This chapter highlights the basic theory of membrane process and the types and mechanisms of transport phenomenon, and it provides a critical analysis of the RO process.

3.2 OVERVIEW OF MEMBRANE PROCESSES

A membrane process can be defined as a process with different types of membrane modules which separate impurities or particles of different sizes from gas and liquid mixtures by allowing or disallowing the selective passage of some particles through the membrane under given operating parameters. Membranes are made of different structures (porous or non-porous) and materials (organic or non-organic). In general, a membrane can be considered as a barrier (intervening phase) between two phases, where the separation takes place given the pressure, concentration, or temperature differences between the two sides of the membrane. This technology has been widely used in several applications, such as seawater desalination, wastewater treatment, and the biotechnology, pharmaceutical, and food industries.

Membrane separation technology and especially the RO process have been progressively used in seawater desalination and several industrial practices. This has been achieved with an increasing saving of energy compared to conventional thermal desalination processes based on multi-stage flash (MSF), multi-effect distillation (MED) (Ghaffour et al., 2015), distillation, and liquid-liquid extraction operations. Membrane technology operates at ambient temperature, which reduces the possibility of product degradation. Clayton (2015) confirmed that 65% of desalination plants around the world use RO technology, compared to only 21% using MSF and MED thermal methods. This is mainly due to membrane technology benefiting from simple design and installation and enhanced productivity at reduced energy consumption (Soltanieh and Gill, 1981). Currently, membrane technology offers the cheapest solution for water desalination compared to thermal desalination technologies (Moonkhum et al., 2010; Aghababaei, 2017). Membrane technology and especially the RO process are also used in wastewater reuse and reclamation in several industries (Lee and Lueptow, 2001; Mouiyaa et al., 2018; Cinperi et al., 2019). This

has resulted in an increased investment in wastewater treatment to provide a sustainable secondary reused water source (Farré et al., 2011; Cinperi et al., 2019). However, the long-term reliability of membrane technology in chemical and petrochemical applications is yet to be fully verified. Membrane technology requires several pre-treatment processes due to fouling and membrane scaling issues. This is why several attempts have been made to improve the synthesis of membranes, including especially the development of chemical and thermally stable membranes characterised by improved performance with reduced fouling (Ahmed et al., 2018; Galiano et al., 2018). The permeation and performance enhancement of RO membranes, however, remains a key challenge and requires further research (Fuyuki et al., 2009; Otitoju et al., 2018).

3.3 TRANSPORT MECHANISMS

For the purposes of developing new types of high-efficiency membranes, the importance of knowing the transport mechanism through the membrane is critical. The most important separation techniques that occur in membranes are the permeability and diffusivity of both the solvent and solute through the membrane. The transport of fluid molecules in open channels and porous media takes place as a result of convection, dispersion in porous media, and diffusion (Strathmann et al., 2011). The convective transport is due to pressure gradient, while the molecular transport is proportional to turbulence intensity. The dispersion is dependent on membrane pore sizes. The molecules at the bulk fluid are transferred from a higher concentration region to a lower concentration region by diffusion, which is dependent on the concentration gradient. However, the operational time, temperature, osmotic and hydrostatic pressure pH, membrane structure and pore size, and fouling affect the permeability of the membrane (Michalov, 1989). Generally, the water is permeated through the membrane and leaves the solute to accumulate on the solution-membrane boundary layer. Then, the solute diffuses back to the solution thus forming a concentration gradient in the boundary layer. This forms a significant layer of solute, which is known as concentration polarisation. In essence, the permeated water is a consequence of interaction of several variables such as concentration, pressure, and temperature gradients. In contrast, the pore size of the membrane can determine the rate of the membrane diffusivity (Soltanieh and Gill, 1981).

The mechanism of transport through the membrane can be explained by two main theories based on two sets of assumptions. For porous membranes, the transport between the feed and permeate takes place through the pores themselves, which run the length of the membrane barrier layer rather than the dense matrix of the membrane. According to this assumption, the transport occurs by both the diffusion and the pressure-driven convective flow through the pores (Baker, 2012). In this type of membrane, the particles with sizes bigger than those of the pores will not be allowed to pass (are excluded) through the membrane. In contrast, for non-porous membranes (homogeneous membrane), the transport takes place through a special mechanism known as solution-diffusion mechanism through polymer chains. Basically, both the solvent and the solute are dissolved into the membrane and diffused across it down a concentration gradient to the permeate side. The main key difference in this transport

through this type of membrane is the solubility of the molecules in the membrane, which vary depending on the type of membrane materials (Lonsdale et al., 1965).

3.4 TYPES OF PRESSURE-DRIVEN MEMBRANE PROCESSES

Four categories of pressure-driven membrane filtration processes are used in both seawater desalination and wastewater treatment. They include microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO). The filtration processes are mainly distinguished by the pore size of the membrane. The largest pore size is found in microfiltration, followed by ultrafiltration, nanofiltration, and the RO process, with the smallest pore size. The fundamental principle of these membranes is that it prevents the passage of particles of sizes bigger than those of the membrane pores and allows the smaller particles to pass through the membrane (Cheryan, 1998). The filtration processes are also distinguished based on the size of ions, molecules, and suspended particles that either are permitted to pass through the membrane or are retained at the membrane surface. Specifically, MF and UF are used to remove particles, while NF and RO are used to remove ions and molecules from water. Generally, all the aforementioned technologies can be differentiated further based on their operating transmembrane pressure difference, solute rejection, and recovery rate. Typically, RO and NF membranes are designed as spiral wound, whereas hollow fibre and high transmembrane pressure is used for such processes leading to high solute rejection. MF and NF membranes can also be designed as hollow fibre, with low transmembrane pressure used to achieve the filtration (Cheryan, 1998). In an RO process, water passes in crossflow through the molecular structure, whereas in UF, water passes through discrete pores in dead-end flow. Table 3.1 shows the four membrane techniques together with the ranges of applied pressure and the associated limitations of their pore sizes (Hendricks, 2006; Paulen and Fikar, 2016).

The table clearly shows that an RO process can eliminate smaller size pollutants, which is not possible to be removed by the MF or UF membranes. RO membrane pore size ranges from 0.1 to 1.0 nm, which enables it to be used as a superior treatment method in several industrial applications.

The next sections deal with the description and characteristics of the main two types of pressure-driven membrane processes: NF and RO.

TABLE 3.1
Specifications of Membrane Types

Membrane type	Pore size (µm)	Applied pressure (atm)
Microfiltration	0.1–2	0.335–2.013
Ultrafiltration	0.01–0.1	1.006–4.026
Nanofiltration	0.001–0.01	5.368–6.711
Reverse osmosis	0.0001–0.001	9.869–98.692

(Adapted from Hendricks, 2006; Paulen and Fikar, 2016)

3.4.1 NANOFILTRATION (NF)

Nanofiltration is a type of pressure-driven membrane process which is between UF and RO membrane processes. NF membranes are usually used to treat a variety of different waters, including surface, ground, and waste, to remove hardness, turbidity, microorganisms, organics, and dissolved salts. The biggest advantage of this process is its high flux at low operating pressure leading to high removal of multivalent anion salts. This is why this low energy consumption technology is used as a pretreatment step in many desalination plants to degrade the ionic strength of aqueous solutions (Hilal et al., 2004). However, its applicability for removal of dissolved salts is lower than that of an RO process.

3.4.2 REVERSE OSMOSIS (RO)

RO is a pressure-driven membrane process, which uses a synthesised semi-permeable membrane made from cellulose acetate and polyamide to separate two mediums of different solute concentration. The membrane allows the solvent to permeate while the solute is retained/rejected by the membrane. Therefore, an RO process can be used to retain undesirable elements such as salts and pollutants from different types of liquid solutions such as seawater and wastewater. The filtration process starts by pumping the solution inside a closed vessel at higher pressure than the osmotic pressure. This aids the water to flow through the membrane from the high-concentration side to the low-concentration side. This process produces two streams of different characteristics. The high-concentration stream is discharged outside the process as brine, while the high-quality water passing through the membrane is discharged as permeate of low concentration.

Figure 3.1 shows a schematic diagram of natural and reverse osmosis processes using semi-permeable membranes. The natural osmosis is represented in scenario

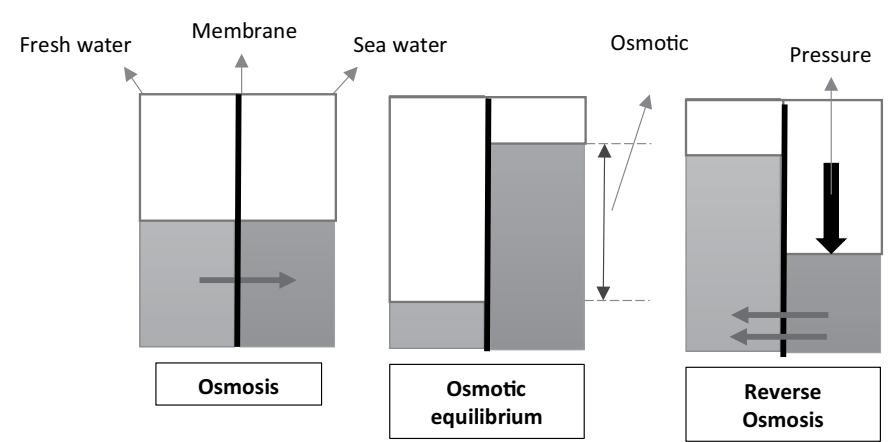


FIGURE 3.1 Scenario A: osmosis; scenario B: osmotic equilibrium; and scenario C: reverse osmosis.

A, where the water diffuses from the low-concentration solution to the high-concentration solution. The natural osmotic movement of the water molecules is essentially driven by the chemical potential of both solutions and continues until osmotic equilibrium is attained because of equal chemical potential for the two separated solutions. From this point onward, the osmotic pressure difference between the two solutions prevents any further solvent flow from taking place. This is represented in scenario B and known as the osmotic equilibrium state. Applying higher operating pressures in excess of the osmotic pressure difference forces the water to flow from the high-concentration solution to a region of low solute concentration. This is ensured with retaining the dissolved salts on the membrane surface to accomplish the main idea of water desalination and is represented in scenario C. Jian and Gupta (2004) confirmed that the water desalination by RO process is mainly carried out at ambient temperature and without any phase change, unlike other thermal desalination processes.

The RO process has several immediate advantages such as high packing density, minimum thermal damage, no chemical reactions, low energy consumption, and high rate of pollutant removal (Fritzmann et al., 2007; Reverberi et al., 2014). The RO process offers both sustainable and economical solutions for seawater desalination with high-quality fresh water at low capital and operating costs (Marcovecchio et al., 2005). The RO process is now widely used to reclaim wastewater from several industrial wastewater effluents (Blandin et al., 2016). However, the disposal of highly concentrated streams of the RO process is still an environmental problem in several applications.

3.5 RO PROCESS PERFORMANCE MEASURES

The performance of RO process can be measured by:

- Transmembrane pressure and osmotic pressure: the transmembrane pressure is an important parameter that represents the driving force of water flow through the membrane. In this respect, the feed pressure is adjusted to overcome the summation of osmotic pressure (dependent on feed solute concentration), friction losses, membrane resistance, and permeate pressure, which assures the economical water passage through the membrane.
- Water recovery: this denotes the total permeate flow rate that can be produced from the total feed flow rate.
- Solute rejection: this expresses the process performance and especially membrane characteristics for the removal of solutes from an aqueous solution system without phase change. Membrane rejection of micropollutants is known to be based on several parameters, including the following (Bellona et al., 2004; Nghiem and Schäfer, 2005):
 - The physicochemical properties of solutes; this includes solute molecular weight and molecular size.
 - Hydrophobicity/hydrophilicity;¹ highly hydrophilic solutes do not stick to the membrane properly and indeed remain in the water (easily dissolved in water) due to their high hydrophilicity. Therefore, low

membrane rejections can be found for these solutes. Hydrophobicity/hydrophilicity are expressed using $\log K_{ow}$ (Akin and Temelli, 2011).

- The dissociation constant (pK_a).
- The electrostatic repulsion; this is carried out due to different charges (negative membrane surface) that can lead to high pollutants rejection (Bellona and Drewes, 2005).

3.6 TYPES OF RO MEMBRANE MODULES

RO membranes are produced in four types of modules of different configurations, including spiral wound, hollow fibre, tubular, and plate and frame. Each configuration has its unique advantages and disadvantages. The next sections illustrate the background of the two main modules: hollow fibre and spiral wound.

3.6.1 HOLLOW FIBRE MEMBRANE MODULE

This type of membrane module is made from thousands of porous capillary fibres (bundle) (up to 10,000) of the same size (internal diameter of less than 200 μm), which are inserted in a pressure vessel (tubular module) to be pressurised. This has the highest area per unit volume compared to other industrial membrane modules. The process of separation is started by feeding the fluid from a central tube in the unit with a high pressure. The permeate radially flows through the fibres and is collected towards the ends of the module, while the retentate is collected at the other end of the tube. The feed flow in hollow fibre modules is dead-end flow, compared to crossflow in spiral wound modules. This type of membrane has a high packing density, and usually about 50%–60% of the feed can be permeated as fresh water (Khan, 1986). The use of hollow fibre membrane modules has achieved reasonable success in different applications including water desalination, industrial wastewater treatment, and in beverage industries (Paulen and Fikar, 2016). A schematic diagram of the hollow fibre contained in the module housing can be shown in Figure 3.2.

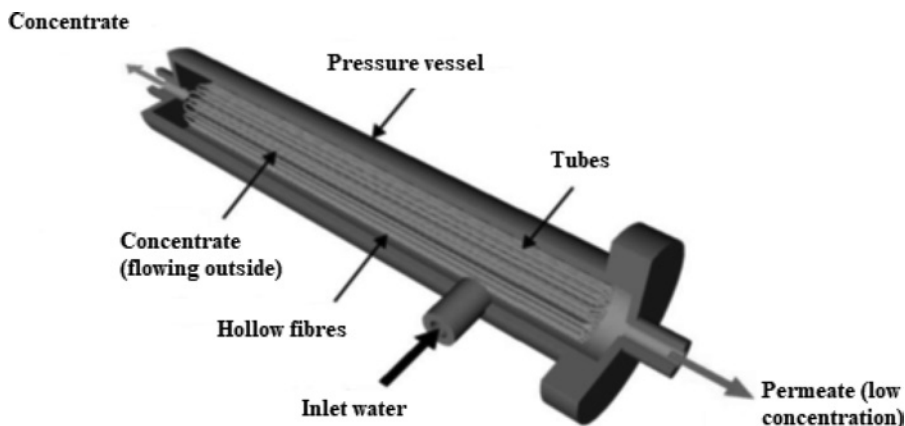


FIGURE 3.2 Schematic configuration of the hollow fibre membrane module.

(Adapted from McMordie Stoughton et al., 2013)

3.6.2 SPIRAL WOUND MEMBRANE MODULE

The spiral wound membrane module is made of several layers of glued flat-rolled membrane sheets wrapped around a central perforated tube to collect high-quality water (Figure 3.3). The spiral wound membranes are put in either a plastic or stainless steel tube to be pressurised. The sheets are bound together around three edges with an opening fourth edge connected with a central perforated tube where the permeated water is collected. The sheets consist of two opposite sides of high- and low-concentration mediums. A very thin fibre mesh of highly porous spacer is used as a barrier to keep the membrane sheets apart, which are wrapped around the perforated tube. This would serve the turbulence intensity inside the module and improve the mass transfer coefficient (Gu et al., 2017). To this extent, the existence of feed spacers reduces the impact of concentration polarisation because of boundary layer degradation at the membrane surface. This is in fact one of the advantages of this module. The process of aqueous solution separation starts by pumping the fluid to impose water flux through the membrane pores. The water flows continuously across the membrane surface (crossflow pattern) at the feed channel. However, the fresh water vertically penetrates the membrane region from the feed side to the permeate side. Thus, the high-quality permeate is collected at the end of the tube at the permeate side. The rate of permeation is related to the pressure gradient between the feed and permeate channels. Also, there is a pressure gradient along the feed channel due to friction. This is why there will be a permeate flow variation along the membrane length.

3.6.2.1 Characteristics of a Spiral Wound RO Process

A spiral wound RO module has several advantages, which promote it as the most popular and often preferred membrane for use in desalination and industrial processes compared to other types of RO membrane modules. Specifically, a spiral wound module comes with a compact design of economical shape of a high packing

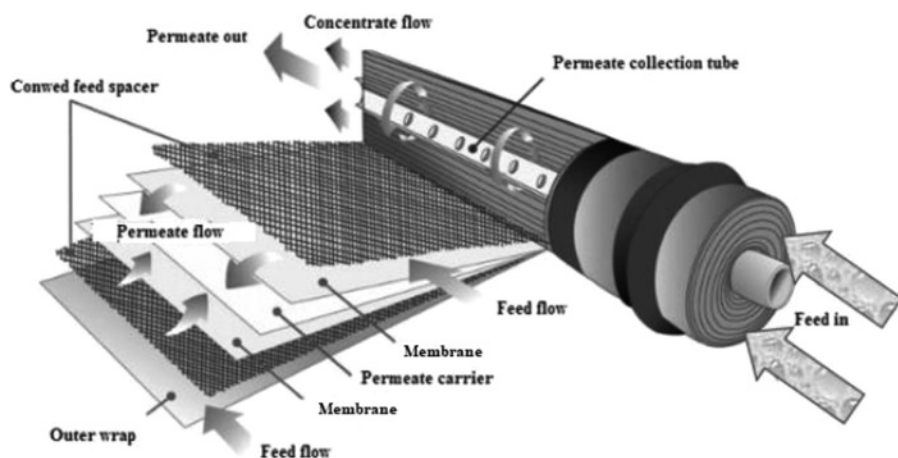


FIGURE 3.3 Schematic configuration of the spiral wound module.

(Adapted from www.complete-water.com/reverse-osmosis-theory-of-operation)

TABLE 3.2
Comparison between the RO Configurations

Module type	Advantages	Limitations	Energy consumption
Spiral wound	Compact, easy to operate Less expensive Good packing density	Plugging Low fouling levels	Moderate
Hollow fibre	Compact Economical High packing density	Plugging	Low
Tubular	Operating at high pressure Easy to clean Resistance to membrane fouling	Plugging	High
Plate and frame	Moderate packing density	Plugging Expensive Difficult to clean	Low to moderate

(Adapted from Baker, 2004)

density (large membrane area per unit module volume). This design facilitates high mass transfer and consumes low energy. Furthermore, this design is characterised by rapid filtration, ease of operation, plausible water flux, low fouling levels compared to the hollow fibre membrane module, and ease of cleaning and replacing at low cost (Song et al., 2002). Also, scale-up of any existing facility can be achieved by additional membranes and pressure vessels.

Table 3.2 provides a brief summary of the advantages, limitations, and energy consumption of the four module configurations, including the spiral wound membrane.

3.6.2.2 Configuration of Spiral Wound Module

A schematic view of the spiral wound membrane element is shown in Figure 3.4 as a flat sheet membrane and includes the directions of water flow inside the module (Al-Obaidi et al., 2017). The membrane length along the x-axis and the width along the y-axis are L and W, respectively. Specifically, x and y represent the axial and tangential coordinates along the length and width, respectively. The membrane is already wrapped in the spiral direction starting from the sealed end of the leaf to the end of membrane width. Therefore, the effective membrane area can be estimated as $A_m = LW$ (t_f and t_p are the height of feed and permeate channels, respectively). The high-quality fresh water is collected at the permeate channel and flows in the spiral direction into a central perforated tube.

3.6.2.3 Limitations of RO Membrane Processes

Membrane clogging, fouling, bacterial growth, and precipitation are the most reported issues of RO technology, and which require pretreatment, periodic cleaning, and flushing. In addition to this, there is an operating lifetime expectancy for any membrane. This dictates the frequency and cost of replacing membrane modules, together with the requirement of using fouling inhibitors and cleaning chemicals such as anti-scalants

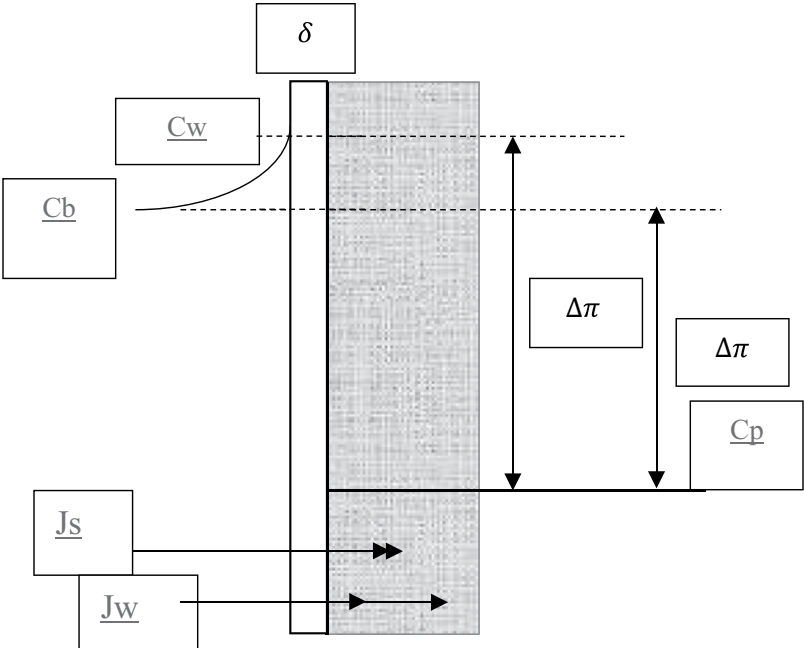


FIGURE 3.5 Schematic diagram of concentration polarisation theory (the bulk concentration (C_b), concentration at the membrane surface (C_w), permeate concentration (C_p), water flux (J_w), solute flux (J_s), and osmotic pressure ($\Delta\pi$).

significantly the mass transfer coefficient. However, this may cause an increase in the energy consumption because of the increased pressure drop along the membrane feed channel (Da Costa et al., 1993). In this respect, Champlin (1998) confirmed that feed spacers could reinforce material deposition due to forming stagnant flow zones behind the feed spacers. Commonly, increasing the operating pressure and temperature can retard concentration polarisation and enhance water flux, especially at low feed concentration and high feed flow rate. Pretreatment also can reduce the concentration of foulants, and it improves filtration performance. However, increasing the feed concentration has the disadvantage of increasing the fouling index due to increasing material deposition at the membrane surface.

3.6.2.3.2 Membrane Fouling

Membrane fouling is an inherent phenomenon and one of the main deficiencies of the membrane technology due to the accumulation of undesirable materials, colloids, and salts on the membrane surface (Chen et al., 2004; Nghiem and Coleman, 2008). Also, particles can foul membranes as a result of pores being blocked due to surface deposition and gel polarisation. This can cause a significant decline of water flux through the membrane and degradation of the membrane performance, especially for high-concentration feed compared to no fouling conditions (Barger and Carnahan, 1991; Xu et al., 2006; Agenson and Urase, 2007). The high-concentration

feed causes a noticeable increase in the osmotic pressure and the hydraulic resistance, which increases the pressure drop along the membrane length. Higher operating pressures are therefore required to settle out this concern, which unfortunately also means higher energy demand and a reduced lifetime of the membrane. It is important to note that the degree of fouling is dependent on the water quality and type of chemical and biological matters. For example, Baker et al. (1995) observed a high fouling of biological, organic, and inorganic species of calcium and phosphate with low concentration of aluminium and iron when treating a polluted surface water using spiral wound NF membranes. Fouling is a generic problem in membrane filtration and especially in wastewater treatment due to the existence of multicomponent chemicals. Unfortunately, it is not easy to identify the main reasons of fouling in wastewater treatment using membrane technology due to the existence of large amount of impurities of different characteristics (Vincent-Vela et al., 2015). Sassi (2012) confirmed that pretreatment technologies such as coagulation and flocculation followed by filtration media have a positive impact on fouling mitigation. For instance, biofouling of membranes can be reduced by adding biocide and disinfectants such as sodium hypochlorite or hydrogen peroxide (Pervov et al., 2003). Additionally, increasing the turbulent flow regime and recovery, caused by shear-induced motion, can hinder fouling due to transporting particles from the membrane surface to the bulk flow (back transport mechanism). Some types of membrane cleaning can also deter membrane fouling intensity. To remedy this, several attempts have been used for the online monitoring and mitigation of the fouling development in membranes (Ahmed et al., 2018). Other attempts include new developments in membranes with low/no fouling characteristics (Galiano et al., 2018).

3.7 CONCLUSIONS

Membrane technology has been in use for seawater desalination since 1900s. Since then, membrane processes have been used progressively in several applications for seawater desalination, wastewater treatment, and many other applications. This chapter has described membrane technology, different types of membranes, and their advantages and limitations with specific reference to the RO process and spiral wound membrane module.

NOTE

- 1 A hydrophilic molecule is one whose interactions and affinity with water and other polar substances are more thermodynamically favourable than their interactions with oil or other hydrophobic solvents. They are typically charge-polarized and capable of hydrogen bonding. This makes these molecules soluble not only in water but also in other polar solvents (www.assignmentpoint.com/science/biology/hydrophilic.html).

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4 Applications of Reverse Osmosis Process in Wastewater Treatment

4.1 INTRODUCTION

Several industries produce vast amounts of wastewater which they need to dispose of somehow. However, they face increasing challenges for doing this, as such wastewater contains a wide range of complex harmful chemical compounds, which are regulated by strict environmental legislation. Such industries are therefore compelled to use a variety of treatment methods to convert these effluents into high-quality reusable water (Carstea et al., 2016). The pressure on such industries to do better than before is greater nowadays, as many countries have a zero-discharge policy and water prices for industrial use are continuously on the rise.

The use of reverse osmosis (RO) has seen a significant rise in several applications of wastewater treatment for removing several harmful micropollutants, including dissolved organic chemicals, viruses, and toxic compounds. This is a significant change from the past, when RO processes were mainly used to recycle wastewater for reuse in industrial applications such as cooling towers and heat exchangers and in the textile industry (Cinperi et al., 2019). This chapter presents a critical review of implementing the RO process as a wastewater treatment method in several industrial applications, highlighting scopes and limitations. Moreover, this chapter discusses the feasibility and reliability of an RO process in removing a variety of organic and highly toxic compounds from wastewater.

4.2 HISTORICAL EXPANSION OF RO USE IN WASTEWATER TREATMENT

Figure 4.1 shows the historical expansion of the RO process for wastewater treatment, which clearly shows a steady increase since 1977 for facilities used to reclaim wastewater in several industrial applications and demonstrates that RO is gradually becoming the accepted technology in different countries. Figure 4.1 shows the construction of several mega-sized wastewater RO plants with a capacity between 228,000 and 320,000 m³/d as in Kuwait, USA, and Singapore.

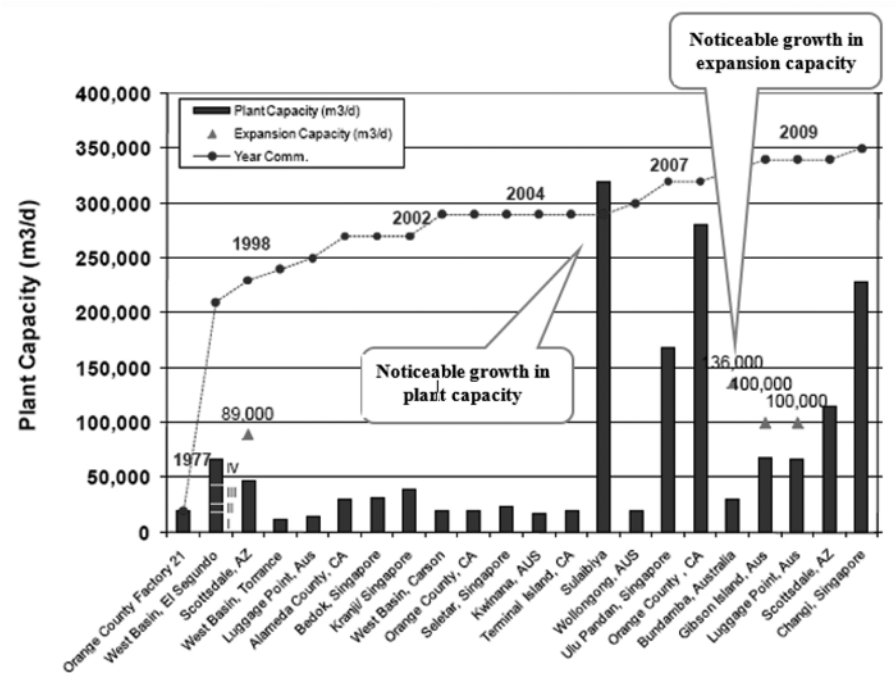


FIGURE 4.1 Historical expansion of RO for wastewater treatment.

(Adapted from Bartels et al., 2010)

4.3 USE OF RO IN WASTEWATER TREATMENT IN SEVERAL INDUSTRIAL APPLICATIONS

RO is considered as one of the pioneering technologies for reclaiming and reusing wastewater effluents of several industries. The semi-permeable membrane aids in removing a wide range of harmful particles and pollutants (Lee and Lueptow, 2001; Akin and Temelli, 2011). Also, an RO process has several advantages, including ease of operation together with high water quality at an acceptable energy consumption (Yin et al., 2018). There exists today a wide market for an RO process capable of treating the effluents of many applications, such as in the tannery industry (Bhattacharya et al., 2013), textile industry (Amar et al., 2009; Cinperi et al., 2019), dairy industry (Koyuncu et al., 2000; Álvarez et al., 2002), and pharmaceutical industry (Gholami et al., 2012). A considerable research effort has been spent to enhance RO use, including maximising the recovery ratio and solute rejection and minimising cost and energy consumption. A number of model-based techniques (modelling, simulation, optimisation) have been used to identify optimal design and operating parameters of the process without resorting to highly expensive experiment-based studies.

The latest research has shown that spiral wound RO processes can offer the best economic and reliable solution compared with RO processes with other membrane

modules. In addition to this, the performance of individual and multi-stage spiral wound RO processes has been assessed by several researchers for industrial wastewater treatment. Such studies involved the evaluation of a wide range of operating conditions for the removal of many chemicals and toxic pollutants from several wastewater effluents. For example, they include a secondary treated sewage effluent (Qin et al., 2005b), a synthetic effluent stream of acrylonitrile, sulphate, ammonium, cyanide, and sodium (Bódalo-Santoyo et al., 2004), di-hydrogen phosphate, sulphite, nitrate, and nitrite (Madaeni and Koocheki, 2010), chromium (Mohammadi et al., 2009), nitrate (Schoeman and Steyn, 2003), copper and nickel (Xijun et al., 1997; Mohsen-Nia et al., 2007), bisphenol A (Khazaali et al., 2014), and industrial wastewater (Gündoğdu et al., 2019). The applications of RO in some of these industries are discussed in the following sections.

4.3.1 TANNERY WASTEWATER TREATMENT

A common effluent of a tannery wastewater treatment plant contains a significant amount of residual organic and inorganic impurities (Bhattacharya et al., 2013). Specifically, a huge amount of chromium is applied in the tanning process of leather, which is then discharged into the sewage system. Tannery wastewater includes various compounds of salt, chromium, suspended solids, surfactants, colours, and fats at high chemical oxygen demand (COD)¹ and biochemical oxygen demand (BOD). The major contaminants include chromium, sulphide, suspended solids, a wide range of inorganic solid waste, and volatile organic compounds (Hassen and Woldeamanuale, 2017). The significant volume of daily tannery discharge of wastewater presents a serious threat to surface water. For example, 50,000 m³ of tannery wastewater is disposed daily into the rivers from Indian leather industries (Dargo and Ayalew, 2014).

The effective conventional treatment methods of tannery wastewater include chemical flocculation and biological processes such as activated sludge process (Ranganathan and Kabadgi, 2011). The RO process is essentially implemented as a successful treatment for reusing tannery wastewater (Purkait et al., 2005; Gisi et al., 2009). For instance, Hafez and El-Mariharawy (2004) used a two-stage/two-pass low-pressure RO membrane design to treat tannery wastewater. They confirmed the possibility of effectively recovering chromium commensurate with the local national limits (<5 mg Cr⁶⁺/l) for discharging into the public sewerage system. However, it is evident that a combination of different technologies (physiochemical pretreatment methods) including coagulation, flocculation, ozone for oxidation, activated carbon for adsorption, and biological treatment (activated sludge process) is more effective for reducing the suspended solids, colour, turbidity, chromium, and nitrogen for treating tannery effluents. This has been confirmed by several studies such as Suthanthararajan et al. (2004), Ranganathan and Kabadgi (2011), Ayoub et al. (2011) and Goswami and Mazumder (2014). These combined technologies do have some disadvantages, including the low efficiency of dropping total dissolved inorganic compounds (Bódalo et al., 2005). This aspect has motivated researchers to investigate the possibility of membrane technology in a hybrid mode in combination with other technologies.

For example, the efficiency of a combination of multi-stage pressure sand filter, filter, photochemical oxidiser, softener, microfilter, nanofilter, and finally a spiral wound polyamide membrane (make: Hydranautics) has been studied by Suthanthararajan et al. (2004) to treat the secondary effluent of tanning industry. It was concluded that an RO membrane system can successfully recover water from secondary-treated tannery effluent, and this yields a considerable amount of permeate that can be reused for the tannery process. Most importantly, the efficiency of the polyamide RO membrane was as high as 98% for removing total dissolved salts (TDS), and where about 94%–98% of Na and Cl ions were also successfully removed.

The performance of a full-scale two-stage/two-pass RO membrane treatment plant of low-pressure RO membrane (LPROM) (7–16 bar) was investigated by Hafez and El-Manharawy (2004) to treat high-concentration chromium Cr^{6+} wastewater. The effluents of two local medium-size tannery shops were considered with chromium concentration varying between 1300 and 2500 ppm and NaCl concentration varying between 40,000 and 50,000 ppm. It is apparent that the RO system used can reduce the chromium concentration to 5 ppm, in line with the national Egyptian limits for discharging chromium into the public sewage system. Bódalo et al. (2005) tested several types of flat low-pressure RO membranes packed in a pressure vessel of a recirculated RO pilot plant (both retentate and permeate recycled to the feed tank) to handle the tanning industry wastewater containing chloride, sulphate, suspended solids, volatile solids, and chromium. The membrane type DESAL-EB was able to reject 98% of impurities based on the conductivity measurements of feed and permeate streams.

Gisi et al. (2009) tested the performance of various treatment methods in tanneries involving a biological pretreatment of a conventional activated sludge process, a physicochemical process using a polymeric coagulant, and finally an RO process. The combined process resulted in a satisfactory removal rate, which is suitable for wastewater recovery and reuse. The results showed a reduction of 67% of COD using the biological pretreatment process. However, the subsequent RO process was able to efficiently reduce the COD further from ammonium substances, resulting in a high-quality permeate. Such an RO process was able to remove the refractory organic compounds of chloride and sulphate efficiently allowing the reuse of wastewater in the tannery production cycle, which resulted in reduced consumption of groundwater. These findings also agreed with the study by Ranganathan and Kabadgi (2011), who considered five conventional tannery plants, where chemical coagulation and biological treatment were used followed by an RO membrane process to treat the wastewater effluents. Finally, Bhattacharya et al. (2013) used a dual stage of micro-filtration and RO membranes to treat highly contaminated organic and inorganic tannery wastewater from common effluent treatment plants. Basically, the permeate of MF was reprocessed in RO as a second treatment step. It was concluded that an RO process can remove 99% of total organic compounds and 82% of sodium. Accordingly, the RO membrane technology has confirmed its suitability for efficiently treating the effluents of tanning industries.

4.3.2 TEXTILE WASTEWATER TREATMENT

The textile industry consumes large amounts of water and therefore produces large quantities of wastewater from different stages of dyeing, rinsing, bleaching, and

finishing processes. The wastewater contains a variety of high levels of COD salts, effluent organic matters surfactants, and dyes; all of which have a significant impact on the ecosystem (Altinbas et al., 1995; Yin et al., 2018). Membrane technology and specifically RO processes are the most popular technologies used in the treatment of wastewater from textile industries (Kabdasli et al., 2000; Dhodapkar et al., 2007). RO processes are used in combination with other conventional technologies to enhance the treatment process. For instance, the biological treatment process by activated sludge offers high efficiency in COD removal but does not completely remove the colour and water salinity (Pala and Tokat, 2002). The physicochemical methods used can remove suspended pollutants but only at high chemical cost and lower soluble COD and salinity removal efficiency (Marrot and Roche, 2002). Several attempts can be found in the literature which assessed RO process efficiency in textile wastewater. Some of such examples are discussed in the next sections.

Treffry-Goatley et al. (1983) tested a pilot plant containing screening, alum coagulation, microfiltration, and two-stage RO membranes to treat cotton/nylon/polyester dye-house effluents. They noticed that 97%–99% of TDS and sodium, 90%–94% of colour, and 88%–97% of COD were removed by the RO system. This is a promising performance, and one that is in line with 85%–95% total water recovery, 65% of organics, 81% ADMI colour, and 100% suspended solids removed by microfiltration. Ciardelli et al. (2000) used membrane technology of spiral wound ultrafiltration and RO process with ozone treatment followed by the pretreatment steps of coagulation, sand filtration, and disinfection processes for the purification of textile and dyeing wastewater for reuse. The individual RO process used confirmed 95% of salt removal and almost 100% COD and colour removal.

Dhodapkar et al. (2007) considered tertiary effluents treated by a physicochemical and biological activated sludge process in advanced treatment processes of a multi-grade filter, ultrafiltration (UF), and RO. The RO process was able to produce reusable boiler water from tertiary treated textile wastewater in line with the regulations of the Indian Standards Institution. Moreover, Chang et al. (2009) used a hybrid system of ozonation, UF, and RO processes to treat the wastewater of a textile plant. This also affirmed the high-quality reuse water in line with the regulations for direct discharge or reuse of wastewater.

Lu et al. (2010) used a pilot plant combining biological treatment with membrane technology to treat textile industry effluents of several types of dyes, sulphide, detergents, solvents, inorganic salts, and heavy metals. These experiments confirmed the reduction/removal of 93%, 94.5%, 92.9%, and 100% for COD, colour, turbidity, and suspended solids, respectively.

Another experimental study (Liu et al., 2011) was carried out to test the performance of nanofiltration (NF) and RO to treat biologically treated textile effluents. This study confirmed that both NF and RO membranes could successfully reduce/remove the COD, BOD, colour, and salinity, and that the hydrodynamic conditions played important roles in flux performances of the membrane. However, the performance of an RO process proved to be more efficient for removing dissolved salts than an NF membrane did.

Kurt et al. (2012) used a pilot-scale NF and RO membrane system in different modes of batch concentrate-recycle mode and continuous mode without concentrate recycle to treat and decolourise segregated wastewaters from dye wash processes

in a weaving industry. Their main aim was to reduce/remove COD and salts. The experiments during the batch operation of the retentate recycling mode confirmed COD reduction of $98.4\% \pm 2.2\%$ to $99.6\% \pm 0.7\%$, colour removal of $98.6\% \pm 1.5$ to 100% , and conductivity reduction of $66.4\% \pm 4.4\%$ to $96.4\% \pm 2.0\%$ for NF and RO, respectively. Similar results were obtained during the continuous operation mode.

4.3.3 ELECTROPLATING WASTEWATER TREATMENT

The electroplating industry also generates large amounts of wastewater which contains heavy metals and is harmful to the environment. Specifically, the plating process is repeated in bathing cycles, which causes a contamination of water in rinsing baths. Therefore, several organic and heavy metals can be found, such as chromium, zinc, copper, nickel, lead, iron, cations, and anions, including oil and grease (Qin et al., 2010). Conventional methods used for removing heavy metals from industrial effluents include precipitation, ion exchange, adsorption, and evaporation (Ku and Jung, 2001). However, the treated effluents still had a high portion of heavy metals, which require a suitable treatment prior to discharge into natural resources (Srisuwan and Thongchai, 2002). The other complication here is that insoluble precipitates may be formed during the precipitation processes (Fu and Wang, 2011). Interestingly, the RO membrane technology has proved to be more effective than other methods for treating such wastewater.

An RO process is usually selected as a final treatment step to improve the quality of the electroplating effluents. For instance, Xijun et al. (1997) confirmed the high rejection of copper from an electroplating wastewater using a pilot scale of two membrane modules in series of a spiral wound RO process. Also, Benito and Ruiz (2002) studied the efficiency of two lines of a spiral wound RO process to reduce the concentration of pollutants found in the electroplating industry. Their results showed nearly total removal of metals in the permeate.

Petricin et al. (2015) tested the merits of combining UF and RO processes to treat the electroplating industry effluents, where UF is used as a pretreatment step to remove dissolved and colloidal contaminants. This would mitigate the fouling propensity in the RO process. Specifically, this combination removed between 91.3% and 99.8% of metal elements and organic and inorganic contaminants from the effluents. More importantly, all suspended solids, ammonium, nitrogen, nickel, sulphate nitrogen, COD, and BOD were totally removed.

4.3.4 PHARMACEUTICAL WASTEWATER TREATMENT

The pharmaceutical industry has received comparatively little attention as a source of generating harmful substances discharged in the environment, despite pharmaceuticals having a direct biological impact on microbes (Dolar et al., 2011). The effluents of pharmaceutical industries are characterised by high organic matters and salt compounds, toxicity, and deep colour (Gholami et al., 2012). Unfortunately, many pharmaceutical substances harmful to humans and animals are partially discharged directly into the sewage system and natural water resources, depending upon the physiochemical properties (Al-Rifai et al., 2007). In this respect, Kemper (2008)

confirmed the existence of more than 30 pharmaceutical substances and their metabolites in sewage influent and effluent samples of water sources including groundwater, drinking water, and surface water. This means that pharmaceutical effluents are not sufficiently treated before they are discharged into our natural aquifers. This, in turn, has led to an increase in attempts to implement a more effective treatment method (such as an RO process) for pharmaceutical wastewater. For example, the efficiency of two high-pressure RO membranes to remove selected veterinary pharmaceuticals and antibiotics was analysed by Dolar et al. (2011). The experiments showed an excellent removal rate of selected pharmaceutical compounds. Moreover, the efficacy of a pilot-scale low-pressure spiral wound RO membrane for the removal of selected antibiotics (ampicillin and amoxicillin) from synthetic wastewater was studied by Gholami et al. (2012). Results showed a range of rejection percentage from 73.52% to 99.36%, and 75.1% to 98.8% for amoxicillin and ampicillin, respectively.

Another study carried out by Kimura et al. (2003) described a feed of 100 ng/l each of bisphenol A, phenacetine, and primidone, which has been tested in a bench-scale filtration system of a flat sheet NF membrane and ultra-low-pressure RO membrane. This study also confirmed that the RO membrane had a higher rejection rate compared with the NF membrane (Table 4.1), and this was mostly due to the pore size impact and the size of tested compounds.

In the same context, the performance of high-pressure polyamide and cellulose acetate RO membranes has been by tested by Kimura et al. (2004). This was based on a bench-scale crossflow experiment for removing 11 neutral (uncharged) endocrine-disrupting chemicals (EDCs) and pharmaceutically active compounds (PhACs) (Table 4.2). The results clearly show that polyamide RO membranes are generally effective for reducing the selected toxic contaminants compared to the cellulose RO membrane.

Broadly speaking, the molecular weight cut-off (MWCO)² can be used as a guide to indicate the extent of micropollutant removal by RO membranes and for recognising their usefulness in a certain separation process (Davey et al., 2017). Therefore, the highly efficient removal of polyamide membranes can be attributed to the interrelation that exists between the molecular weight of the specified compounds and its removal based on the theory of size exclusion. However, the polarity can identify the rejection in cellulose membrane type as a dominant reason for the removal of

TABLE 4.1**Comparison of NF and RO Rejection in Pharmaceutical Wastewater**

Toxic contaminant	Rejection by NF membrane (ESNA) (%)	Rejection by RO membrane (RO-XLE) (%)
2-Naphthol	12	43
Bisphenol A	45	99
Primidone	87	84
Phenacetine	19	71

(Adapted from Kimura et al., 2003)

TABLE 4.2
Rejection of Toxic Several Pharmaceutical Contaminants
by Two RO Membranes

Toxic pharmaceutical contaminants	Rejection by polyamide membrane (XLE) (%)	Rejection by cellulose membrane (SC-3100) (%)
Bisphenol-A	83	18
Caffeine	70	44
Carbamazepine	91	85
Isopropylantipyrine	78	69
NAC standard	79	0
Phenacetin	74	10
Primidone	87	85
Sulphamethoxazole	70	82
2-Naphthol	57	0
4-Phenylphenol	61	11
17β-Estradiol	83	29

(Adapted from Kimura et al., 2004)

such compounds. Nevertheless, the polyamide membrane shows a rejection range of 57%–91% only. One of the conclusions of the Kimura et al. (2004) study is that the rejection of micropollutants in an RO membrane is entirely dependent on the properties of both the membrane and the specified compound. Moreover, this study also confirmed that MWCO is not the best tool for predicting more precisely the rejection of micropollutants and specially EDCs/PhACs by RO membranes (Bellona et al., 2004).

4.3.5 OILY WASTEWATER TREATMENT

The fast-growing oil and gas, petrochemical, pharmaceutical, and food industries produce vast amounts of oily wastewater. This harmful and toxic industrial wastewater can exist in various types such as free, dispersed, emulsified, and dissolved oils (based primarily on size) (Rhee et al., 1987). It also includes a wide range of hazardous petrochemical organic compounds and aromatic hydrocarbons such as benzene, toluene, naphthalene, xylenes, phenols, benzofluorene, and pyrene at variable concentrations (Benito-Alcázar et al., 2010). However, the refinery process water generally encompasses less dissolved inorganic ions. The mutagenic and carcinogenic organisms contained in such wastewater require treatment before the wastewater can be safely disposed of into ground or water resources. In contrast, oily wastewaters can be used in cooling tower systems in oil refineries but require a pretreatment (Li et al., 2006). This usually comprises a set of physical, chemical, and biological water technologies treatment applications. Specifically, it includes adsorption, gravity separation, skimming, sand filter, dissolved air flotation, de-emulsification, coagulation and flocculation, heating, centrifugation, precoat filtration, fibre beds, and electrochemical methods (Munirasu et al., 2016). In this respect, Cheryan and

Rajagopalan (1998) and Padaki et al. (2015) demonstrated several limitations of conventional methods. They include large space treatment plants, production of a high quantity of sludge, corrosion and mechanical problems, increased dissolved solids content in the effluent, and high operation and energy cost. On the other hand, the use of a low-energy and low-cost RO membrane technology has proved its merit for being used as an alternative method for treating oil water emulsions. This is largely due to its ability to remove high oil droplets more effectively compared to conventional methods (Padaki et al., 2015).

Among all the membrane processes, UF was found to be the best method to effectively treat oily wastewater (He and Jiang, 2008). However, RO and NF are more efficient than UF if the oily wastewater has a high concentration of salt (Cheryan and Rajagopalan, 1998). However, fouling and degradation remain as the key challenges for polymeric membranes used for oily wastewater. Unfortunately, these require frequent replacement, an aspect that can significantly increase operating costs. Moreover, the hybridisation of membranes with conventional chemical treatment systems can also be useful to concentrate sludges (Cheryan and Rajagopalan, 1998). Several examples of the implementation of RO process to treat oily wastewater can be found in the literature.

Norouzbahari et al. (2009) examined the effectiveness of a hybrid hydrophilic flat sheet polysulphone UF membrane and spiral wound thin-film composite polyamide RO membrane separation process to treat crude oil desalter effluent from an Iranian oil refinery. In this respect, more than 95% of TDS was removed by RO.

Salahi et al. (2012) studied the practical feasibility of using an RO membrane to treat Iranian refinery wastewater of 1953 TDS. This included the investigation of membrane performance at 8, 15, and 20 bar of transmembrane pressure, 0.5, 1, and 1.5 m/s of feed velocity, 4, 7, and 10 pH, and 27.5, 37.5, and 50 °C of operating temperature. The investigation confirmed a positive influence of the parameters studied on the permeation flux, except pH. More importantly, the permeate quality of 253 of TDS was confirmed, denoting a good water quality. The findings also highlighted a high reduction of COD (95%), biochemical oxygen demand (95%), total organic carbon (TOC) (90%), TDS (87%), oil and grease content (87%), and turbidity (82%). Moreover, the treatment achieved total removal of colour, free oil, and total suspended solids (TSS) with a plausible permeate flux of 50 l/m² h.

Clearly, the combination of several treatment methods yields better results when treating oily wastewater due to the presence of complex compounds. Vincent-Vela et al. (2015) studied the feasibility of recovering effluents of a petrochemical industry using a combination of different pretreatment processes including coagulation–flocculation process, MF, and UF to attain an appropriate feed effluent for the RO process. The study confirmed a significant removal of suspended solids (SS), turbidity, and COD. This in turn showed the feasibility of this hybrid system to meet the requirement for discharge and produce water that can be reused.

4.3.6 PULP AND PAPER WASTEWATER TREATMENT

The pulp and paper industry also produces a vast amount of inorganic and organic constituents of bleach effluents. Specifically, the bleach effluents have high biochemical oxygen demand, chemical oxygen demand, suspended solids, toxicity, and colour

(Kamali and Khodaparast, 2015). More specifically, the wood industry produces high concentrations of chlorides, phenols, terpenes, resin acids, non-biodegradable matters, and lignin degradation products (Simpson and Groves, 1983; Buyukkamaci and Koken, 2010). In addition, the pulp industry consumes large quantities of water, which requires suitable treatment methods for recycling and reusing wastewater (Saif et al., 2012). Several treatment methods have been applied to degrade the existence of these pollutants, such as the physicochemical treatment (sedimentation, flotation, coagulation and precipitation, adsorption, chemical oxidation, ozonation, electrolysis, and membrane technology), biological treatment, fungal treatment, and hybrid treatment processes (Kamali and Khodaparast, 2015).

Among all the previously mentioned processes currently used for pulp and paper bleach treatment, the low-cost membrane technology and especially the RO process have shown great success for removing over 90% of colour, total suspended solids, chlorinated phenolic compounds, and adsorbable organic halides (Pokhrel and Viraraghavan, 2004). Also, the RO process used confirmed its ability to destroy pathogens (Asano and Cotruvo, 2004). This means that an RO process is capable of removing both inorganic salts and low molecular weight organic compounds at moderate temperature and a wide range of pH. This is why RO processes have become the most acceptable method in the pulp and paper industry, especially in combination with other physicochemical processes to achieve a high removal of toxic micropollutants. For instance, Pizzichini et al. (2005) tested several types of membrane modules, including spiral wound RO membrane, to treat the wastewaters of an Italian paper mill that employed recycled paper. The goal was to produce a good-quality permeate and minimise the process energy consumption by manipulating the operating parameters of transmembrane pressure and feed flow rate at fixed temperature. A combination of MF and RO processes yielded the removal of the dissolved solids at a rate of 965–99% with no heavy metal in the permeate.

Li and Zhang (2011) concluded the possibility of reducing COD by around 75% satisfying stringent environmental regulations if a composite flocculant is used as a pretreatment process prior to the RO process in pulp and paper mill wastewater.

Saif et al. (2012) carried out a superstructure optimisation study to synthesise RO network (RON) in order to recycle wastewater streams of a pulp and paper industry while reducing the salt concentration at minimum cost. They were able to achieve recycling of 30% wastewater in the pulp and paper processes. This resulted in a significant reduction of water consumption by around 7700 ton/day with 97% and 98% removal of KCl salts and NaCl salts, respectively.

Kamali and Khodaparast (2015) reviewed the feasibility of several conventional treatment methods used in pulp and paper mill wastewaters and confirmed that the combination of membrane technologies and electrochemical methods can be used as an efficient method for reducing BOD, COD, TSS, and dissolved organic carbon (DOC).

4.3.7 DAIRY WASTEWATER TREATMENT

Dairy industries can be considered as one of the most polluting plants in food manufacturing industries as they use vast amounts of water and produce vast amount of wastewater with a significant amount of pollutants. For example, the dairy sector in

India, being the largest in the world, consumes approximately 62 billion m³ of fresh water every year. According to published statistics, consumption is expected to rise above 400 billion m³ by 2025 (Tiwari et al., 2017; Buabeng-Baidoo et al., 2018). This, in turn, produces a significant amount of effluent, which varies from 0.2 to 10 litres of effluents per litre of processed milk. Such quantities are produced during the starting, equilibrating, interrupting, and rinsing steps. Smithers (2008) and Bharati and Shinkar (2013) reported approximately 6 g/l of COD from the high concentration of organic matter in dairy wastewater, which requires appropriate treatment methods. Membrane technology and especially the RO process have been considered by Balannec et al. (2005) and Vourch et al. (2005). This process produced a high-quality permeate as purified water for reuse and has helped reduce water consumption in the dairy plant.

Koyuncu et al. (2000) explored the efficacy of membrane technology for treating and reusing wastewater of the dairy industry from an existing chemical and biological treatment plant. This included the use of two-pass low-pressure spiral wound RO membranes of close recycle system (retentate and permeate are recycled to the feed tank). The two-pass system involved the permeate of the first RO membrane to be used as the feed for the second RO membrane. The experiments were carried out at 27 °C and at 6, 10, 14, and 18 bar pressure with 2000–10,000 ppm of inlet COD, 1800 µS/cm of conductivity, and 790 ppm of suspended solids. They achieved a high-quality permeate with a 98%–99% reduction of COD, conductivity, and SS.

Vourch et al. (2005) used a two-stage spiral wound membrane treatment of RO process to concentrate dairy matter and produce reusable purified water. The performance indicators of milk components rejection, permeate flux, and purified water characteristics were taken into consideration. The filtration experiments were carried out at 20 bar, 800 L/h, 25 °C of pressure, flow rate, and temperature, respectively. The RO membrane treatment was found to produce highly purified water, satisfying TOC drinking water regulation for reuse in the dairy industry.

Balannec et al. (2005) applied RO membranes to concentrate diluted skimmed milk. The permeate quality was measured based on COD. The experiments were carried out in a stainless steel cylindrical batch cell at 25 bar pressure and 25 °C temperature. They observed that a single step of RO membrane was insufficient to produce permeate with the required COD for human consumption. This was also investigated by Balannec et al. (2002), who suggested that a further RO step might be used to refine the permeate further and render it a reusable water.

Vourch et al. (2008) studied the efficiency of a spiral wound RO membrane (2.5 m²) in a crossflow filtration system for treating several selected wastewaters from 11 French dairy plants for water reuse purposes. To recover 90%–95% water, 20 bar, 25 °C, and 800 L/h of pressure, temperature, and flow rate were used. The removal efficiency was found to be high for all tested compounds. Specifically, more than 99.8% and 99.5% of TOC and lactose (organic matter), respectively, were removed. Also, nitrogenous compounds and conductivity were reduced by around 96% and 97%, respectively.

Suárez et al. (2014) used a spiral wound RO membrane for treating low-pollutant dairy condensates from flash coolers of an ultra-high-temperature (UHT) process of a dairy plant. The aim was to generate high-quality boiler water. Depending on the

process operating conditions, the experiments depicted the possibility of reducing up to 98.2% and 97.8% of conductivity and chemical oxygen demand, respectively.

The effectiveness of a double-stage integrated filtration system of microfiltration and RO membranes for treating dairy wastewater has been evaluated by Bortoluzzi et al. (2017). They reported a significant removal of total solids and organic matter of 100% turbidity, 100% colour, 94% total Kjeldahl nitrogen (TKN), and 84% total organic carbon. They explored the possibility of using reused wastewater in the cooling and heating processes of the dairy plant.

Finally, Buabeng-Baidoo et al. (2016) studied water reuse/recycle opportunities in a large-scale milk processing plant through process integration based on a comprehensive superstructure optimisation. A comprehensive regenerator model (hollow fibre RO process) was embedded within a WN (water network) model. They observed that water integration coupled with an RO regeneration system led to a significant reduction in freshwater consumption and wastewater generation.

4.4 USE OF RO IN SMALL- TO LARGE-SCALE WASTEWATER TREATMENT PLANTS

The next sections highlight the performance analysis of the RO process as a prominent treatment method in both pilot-scale systems and large-scale wastewater systems while removing pollutants using various types of commercial membranes.

4.4.1 PILOT-SCALE WASTEWATER SYSTEM

The efficiency of a pilot-scale filtration batch system of a flat cell RO module provided by INDEVEN (Spain) was tested by Bódalo et al. (2004) for treating a multicomponent synthetic effluent of inorganic species of ammonium, sulphate, and cyanide compounds. The experiments were carried out at different feed concentrations and confirmed the rejections of 92.7%–93.5%, 93.8%–93.9%, and 88%–90% for ammonium, sulphate, and cyanide, respectively.

The effect of membrane type and operating parameters on the efficiency of a bench-scale flat sheet membrane (3E-3 m²) for treating aqueous solutions of aniline was explored by Gómez et al. (2009). The membrane HR98PP type was found to have the highest rejection of 91.8% of aniline compared to the MS05 membrane, which achieved the lowest rejection of 79%. Also, it was concluded that increasing the operating pressure would slightly improve aniline rejection.

Sagne et al. (2010) studied the impact of membrane type and operating parameters on the performance of an RO pilot plant of an individual spiral wound module (2.6 m²) to remove small organic solutes of carboxylic acids and alcohols from distillery condensates. They found that the membrane type BW30 from Dow yielded a maximum of 80% removal of butyric acid, valeric acid, and 2-phenylethanol solutes compared to CPA2 and ESPA2 membranes from Hydranautics. Moreover, caproic acid and 2,3-butanediol were totally removed.

Thirugnanasambandham et al. (2016) investigated the efficiency of a bench-scale filtration system of a spiral wound RO membrane (2 m²) to treat the wastewater of a wine industry considering a wide range of operating conditions. These have shown

a significant impact on the process performance, notably with optimum reduction of 91%, 93%, and 97% of colour, COD, and TDS, respectively.

4.4.2 LARGE-SCALE WASTEWATER SYSTEM

The RO process has been extensively used in several large-scale municipalities around the world as an effective energy-saving membrane technology in combination with other processes to reclaim wastewaters. The next section discusses two examples of the largest wastewater replenishment plants (Franks et al., 2007) in this context.

4.4.2.1 Orange County Water District (OCWD): Groundwater Replenishment System in California

The OCWD system uses RO to treat secondary effluents from municipal wastewater treatment plants. The final design of the RO system is based on an extensive pilot-scale experimental work of different membrane types within the plant operation. A polyamide RO ESPA2 (8-inch) spiral wound membrane process was used with 15 RO trains in operation and one on standby. Each train includes an array of three-stage 6:4:2 with seven elements per vessel (78:48:24). A stable total water recovery of 85% and total plant capacity of 789 m³/hr at low fouling and energy consumption was achieved. Figure 4.2 shows a schematic diagram of the OCWD plant. Table 4.3 outlines the characteristics of feed water, which shows 1167 ppm, 10.5 ppm, and 2.7 ppm of TDS, TOC, and phosphate, respectively.

The RO process operates at low operating pressure of 9.67 atm (9.8 bar) with energy consumption of 0.41 kWh/m³. The produced water is characterised by 0.3 ppm TOC, approximately 100 ppm TDS, with negligible TSS (www.water-technology.net/projects/groundwaterreplenish/).

4.4.2.2 Ulu Pandan (UP) Wastewater Reclamation Plant in Singapore

Singapore’s UP system uses an RO membrane system to treat secondary effluents from municipal wastewater treatment plants. The final design of the RO system is based on collected experience from two existing wastewater treatment systems in Singapore employing RO membranes. Polyamide RO ESPA2 (8-inch) spiral wound

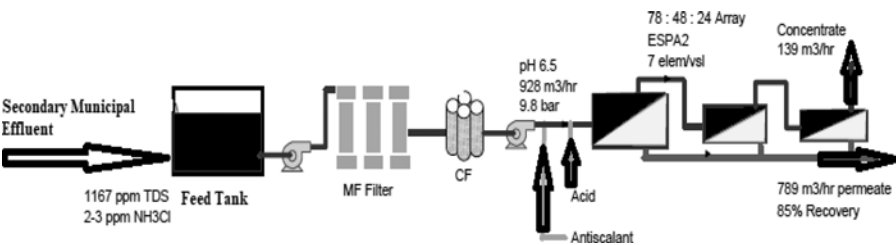


FIGURE 4.2 A schematic diagram of OCWD plant.

(Adapted from Franks et al., 2007)

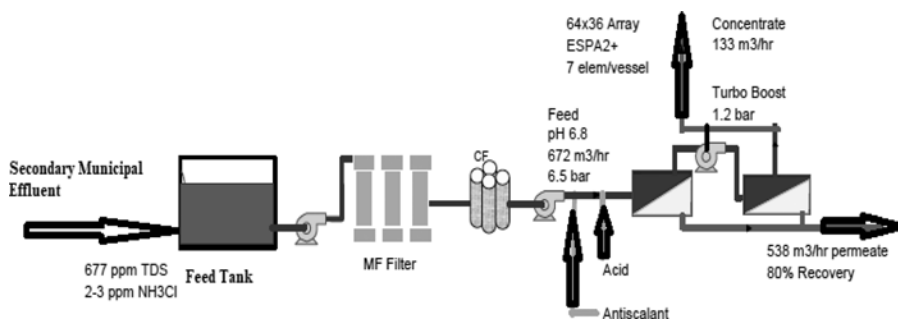


FIGURE 4.3 A schematic diagram of UP plant.

(Adapted from Franks et al., 2007)

RO membrane process consists of 12 trains in operation and one on standby. Each train includes an array of two-stage 4:2 with seven elements per vessel (64:36). A stable RO operation takes place after using anti-scalant, which provides a stable total water recovery of 80% and total plant capacity of 538,000 m³/d at reduced pH of 6.8 and low organic fouling propensity. Figure 4.3 shows a schematic diagram of the UP plant. Table 4.4 outlines the characteristics of feed water, which shows the effluents of 677 ppm, 12 ppm, and 15 ppm of TDS, TOC, and phosphate, respectively.

Interestingly, several aspects reduced the energy consumption significantly to 0.29 kWh/m³ in the plant. They include the low operating pressure of 6.41 atm (6.5 bar), lower feed salinity, greater membrane surface compared to OCWD plant, and the use of an energy recovery device (ERD).

In summary, OCWD and the UP wastewater treatment plant were designed to minimise the total operating cost while producing high-quality permeate. It is worth noting that a high performance of RO process has been observed in both plants in terms of a significant removal of pollutants and low fouling rates.

4.4.3 REMOVAL OF SPECIFIC POLLUTANTS FROM WASTEWATER USING RO PROCESS

This section discusses the removal of certain metals from wastewaters using an RO process.

4.4.3.1 Heavy Metals

Heavy metals have a higher atomic weight than water has, as well as a density that is around five times greater than that of water. Significant amounts of heavy metals have been disposed of into the environment due to rapid urbanisation and industrialisation (Linnan et al., 2009). The existence of heavy metal ions and nitrogenous compounds is considered as one of the main global concerns linked to industrial wastewater. This is because heavy metals are non-biodegradable, unlike organic pollutants. They have a harmful impact on the ecosystem and human life as they can be absorbed by living organisms due to their high solubility in aquatic environments

(Kamitani and Kaneko, 2007; Barakat, 2011). More importantly, heavy metals can be converted to more toxic hydrated ions than can their original version if disposed of into water (Carolin et al., 2017). Heavy metals cause serious health issues such as cancer and organ and nervous system impairment, and they can lead to death (Gunatilake, 2015). This is why there is tighter legislation restricting the discharge of wastewater that contains heavy metals into surface water in several developed countries. For instance, the World Health Organization (WHO), the United States Environmental Protection Agency (US EPA), and the International Agency for Research on Cancer (IARC) have issued severe regulations on discharging heavy metals, specifically chromium, cadmium, arsenic, mercury, and lead, into the ecosystem due to their significant impact on public health (probable human carcinogens) (Tchounwou et al., 2012; Carolin et al., 2017). Consequently, there has been an increased interest to develop a complementary cost-effective treatment methodology for adequately removing these pollutants from wastewater.

Several traditional methods have been used to recover heavy metals from wastewater, such as precipitation, adsorption, ion exchange, evaporation, complexation, and electrochemical processes. However, such methods have proved to be rather expensive due to their high requirements for energy, their unsuitability for completely removing heavy metals, and their ability to form a toxic sludge (Barakat, 2011). Such studies have shown that physical, chemical, and biological treatment methods are not sufficient for removing inorganic heavy metals from wastewater compared to organic pollutants. This is mainly due to the characteristics of heavy metals including solubility, chemical reduction, decomposition, and complex formation (Lee and Dhar, 2012). This is why membrane technology and especially the RO process has provided promising solutions for the treatment and recycling of wastewater in metal plating and aquaculture facilities due to their ability to remove heavy metals and nitrogenous wastes from wastewater with high precision. In addition to this, an RO process would eliminate the shortcomings of other conventional high-cost methods of wastewater treatment (Chai et al., 1997; Qin et al., 2005a; Madaeni and Koocheki, 2006).

Kurniawan et al. (2006) found an RO process to be a superior method for removing heavy metals effectively compared to UF and NF processes. Fu and Wang (2011) reviewed and evaluated several conventional methods used to remove heavy metals from wastewater, including RO processes. They also confirmed the effectiveness of an RO process for successfully removing several toxic metals such as copper, nickel, arsenic, and zinc with a removal rate of 95%–99.5%.

Recently, Carolin et al. (2017) reviewed the fundamental treatment technologies (coagulation/flocculation, ion exchange, flotation, membrane filtration, chemical precipitation, electrochemical treatment, and adsorption) and their efficiency to remove toxic heavy metals from wastewater.

Whilst conventional treatment methods have been found to successfully remove heavy metals from wastewater, they have also been found to have the following disadvantages:

- The coagulation/flocculation method creates a sludge where secondary pollutants can be formed.
- The ion exchange method suffers from fouling.

- The flotation forms an unwanted sludge.
- The membrane requires backwashing.
- The chemical precipitation forms a sludge, which is a problem for low-concentration metals.
- The electrochemical treatment results in a short lifetime of the electrode material.
- The adsorption process can only be useful for laboratory-scale set-ups.

The following sections illustrate the efficiency of RO processes for the removal of well-known toxic heavy metals, including arsenic, aluminium, cadmium, chromium, cobalt, copper, iron, lead, manganese, mercury, molybdenum, nickel, selenium, silver, tin, and zinc from wastewater.

4.4.3.2 Arsenic

Arsenic is a natural and anthropogenic highly toxic and carcinogenic semi-metallic element that can be commonly found in groundwater in several chemical compositions of organic and inorganic compounds such as arsenite and arsenate and at different charges and molecular weight (Durthi et al., 2018). Therefore, several authorities have introduced stringent limits of arsenic contamination in drinking water. For instance, WHO and the US EPA have limited arsenic in drinking water to 10 ppm (Oh et al., 2000). However, the US EPA has issued the maximum contaminated level (MCL) standards of arsenic as 0.05 ppm in 2003 (Babel and Kurniawan, 2004). Several conventional methods are used to lower aqueous arsenic concentration in groundwater, including physicochemical techniques of coagulation and precipitation, adsorption, ion exchange, and membrane technology and biological techniques of phytoremediation and treatment with living microbes/bio-filtration (Song et al., 2006; Mondal et al., 2006; Geucke et al., 2009; Baskan and Pala, 2010). Interestingly, an RO process has been widely used as the main technology for treating brackish water and removing all dissolved species, including iron, calcium, magnesium, bicarbonate, chloride, and sulphate in addition to arsenic (Mondal et al., 2006; Xu et al., 2013). The success of an RO process to remove arsenic is mainly dependent on membrane type and the species of arsenic. However, the membrane fouling remains the key drawback of this technology, especially when iron and manganese are available, but which can be solved by a pretreatment process (Mondal et al., 2006). A bench-scale spiral wound RO process operating at $4.166\text{E-}5\text{ m}^3/\text{s}$, 23.48–25.06 atm, and 25 °C of feed flow rate, pressure, and temperature, respectively, was used by Schneiter and Middtebrooks (1983) to investigate the performance of an RO process for the removal of arsenic from groundwater samples. This showed a 90% removal of arsenic from feed water with arsenic concentrations of 100 µg/L.

Waypa et al. (1997) used bench-scale experiments to study the feasibility of an RO membrane to remove arsenic from spiked natural waters. They found a slight increase in arsenic removal with an increasing pressure from 2.76–27.23 atm. Also, increasing temperature from 15 to 30 °C was found to alleviate the removal of arsenic. A high removal of arsenic of 96%–99% was reported.

Pawlak et al. (2006) tested the performance of a pilot-scale spiral wound RO membrane to reject arsenic from a groundwater source. They reported an effective

and consistent rejection of arsenic at 98.5%. Geucke et al. (2009) tested a small-scale spiral wound RO module on arsenic removal at feed concentrations of 2200 µg/l and 25 °C temperature. The experiments reported a significantly higher removal of arsenate As (V) negatively charged compared to arsenite As (III) neutral charged. This is ascribed to a negatively charge of membrane that promotes the rejection of negatively charged ions such as As (V) due to the charge exclusion phenomenon. Therefore, the selection of negatively charged membranes helped to increase the arsenic removal. More importantly, the permeate contained an arsenic concentration within the recommended limit of 10 µg/l (Sen et al., 2010) by WHO and the US EPA.

4.4.3.3 Cadmium

Cadmium is a bio-persistent (non-biodegradable) heavy metal that can be considered as one of the most ubiquitous and serious environmentally toxic heavy metals. Cadmium can go into wastewater from a variety of applications such as metal and mining, the batteries industry, and electrical cables manufacturing (Filipič, 2012; Carolin et al., 2017). Unfortunately, cadmium is an extremely harmful metal and has therefore been classified as carcinogenic to humans by several regulatory agencies, such as the International Agency for Research on Cancer and by the US National Toxicology Program, even at low concentrations (IARC, 1993; NTP, 2000). The concentration of cadmium is limited at 0.1 ppm by the Tunisian NT106.002 standard when disposed of into the sewer systems (Kheriji et al., 2015), whilst the US EPA has restricted cadmium to 0.01 ppm of MCL standards in 2003 (Babel and Kurniawan, 2004).

A reliable low-cost treatment technology is therefore required for removing cadmium from wastewater. Slater et al. (1987) effectively used a small-scale thin-film composite RO membrane to remove cadmium from industrial waste samples containing several heavy metals and from a single solute system of varied concentrations. More than 99.5% of cadmium rejection was observed at high pressure.

Abu Qdais and Moussa (2004) investigated the performance of a laboratory bench scale of two tubular spiral wound RO membrane (2.5 m²) arranged in series for the treatment of synthetic wastewater samples containing copper and cadmium ions at various concentrations. The experiments resulted in the removal of 98% and 99% of copper and cadmium, respectively, for the same initial concentrations. This clearly shows that an RO process can reduce the heavy metal concentration in wastewater in line with the regulations for industrial wastewater discharge.

Kheriji et al. (2015) studied the major role of two spiral wound RO membranes (0.6 m²) equipped in a pilot plant for the elimination of cadmium ions from wastewater of a battery industry. This study showed that cadmium rejection by RO membranes was more than 90% in the pressure range of 3–15 bar for model water. However, the experiments of industrial effluents containing cadmium showed the highest rejection between 98%–99%. It is clear that the RO process could effectively remove cadmium from the effluent of the battery manufacturing plant within the recommended limits for the disposal of the wastewater.

4.4.3.4 Chromium

Chromium is a steel-grey metallic element used as an important element for plating other metals in semiconductor and electroplating industries. These are considered as

the main sources of chromium contamination in the ecosystem, where the chromium can be released into the environment via leakage or improper disposal practices (Sharma et al., 2008; Mohammadi et al., 2009; Gaikwad and Balomajumder, 2017). Also, leather, textile, and tanning industries are considered as the other sources for disposing chromium into surface water (Atieh et al., 2010; Carolin et al., 2017). A stringent limit of total chromium was recommended by WHO at 50 µg/L (WHO, 2006). However, the Iranian National Discharge Standard has limited the hexavalent chromium concentration in effluent discharge to 0.1 ppm (Mousavi Rad et al., 2009). Also, the US EPA has limited the maximum contaminated level of chromium at 0.05 ppm in 2003 (Babel and Kurniawan, 2004).

Several conventional treatment technologies have been used to remove chromium from wastewater, and they include chemical and electrochemical precipitation, ion exchange, adsorption, and membrane technology (Çimen et al., 2014).

Ozaki et al. (2002) used a crossflow module of ultra-low-pressure flat sheet RO membrane of 60 cm² to treat the wastewater of an electroplating industry, which contains chromium, copper, and nickel. The results of this study confirmed that a high feed concentration generated a high rejection of these metals. However, permeate concentration increased because of increasing feed concentration. Also, increasing pressure caused an increase of permeate flux and ion rejection. More importantly, rejections of 99.37%, 99.03%, and 98.75% of Cr, Ni, and Cu, respectively, were reported. However, rejections of 99.91%, 99.23%, and 99.71% of Cr, Ni, and Cu, respectively, were obtained for the experiments with single metal in the feed solution.

Hafez et al. (2002) studied the chromium removal efficiency from the spent tanning effluent by using pilot-scale membrane units at different salt concentrations and operating pressures. They reported that the chromium removal at 16 bar was up to 99.95% at 1000 ppm of initial chromium concentration and reduced to 98.5% at 4000 ppm.

Mohammadi et al. (2009) investigated the performance of a pilot plant-scale RO process containing a spiral wound module type 2521 TF (Korean CSM company) to remove chromium (Cr⁺⁶) from the effluents of an electroplating industry. The maximum rejection was 99%, and this was achieved at optimum operating conditions.

Mousavi Rad et al. (2009) demonstrated the efficiency of a pilot-scale spiral wound polyamide thin-film composite RO membrane (7.2 m²) for removing hexavalent chromium from an aqueous solution at varied feed concentrations while studying the operating conditions on the process performance at 25 °C temperature. They reported that the permeate flux and water recovery decreased due to increasing feed concentration. Also, a positive impact on pressure has been noted on the permeate flux and recovery. More importantly, the pressure of 18 bar at the lowest feed concentration of 5 ppm gave the highest chromium rejection of 99.8% with permeate concentration of 0.01 ppm and water recovery of 42.47%.

Çimen et al. (2014) investigated the removal of chromium from model solutions containing chromium as a single solute at different operating conditions and 20 °C temperature. In this respect, two seawater and brackish water RO membranes (44 cm²) were used for the separation process. They found that the chromium removal was dependent on the membrane type and actually increased with pressure. The feed

concentration of chromium had no significant impact on the rejection rate and the highest rejection of 95% of chromium was obtained by the RO process.

4.4.3.5 Copper

Copper is non-biodegradable and highly toxic to living organisms, even at low concentrations (An et al., 2014). Copper can be released with the wastewater of electroplating, steel and mining, and paint and fertiliser manufacturing industries as a heavy metal ion, where it has a passive impact on human beings and ocean life (Gao et al., 2013; Awual et al., 2013). Therefore, the recovery of heavy metals and specifically copper from wastewater is very important. Several conventional treatment methods such as sorption, flocculation settling, precipitation, and membrane technology have been used to remove copper from wastewater due to stringent regulations (Cséfalvay et al., 2009). The US EPA has issued the MCL standards of copper as 0.25 ppm in 2003 (Babel and Kurniawan, 2004). The RO process is particularly suited to treat wastewater with low concentration of copper in the effluent of electroplating industries. Example methods are highlighted in the following sections.

Chai et al. (1997) applied a pilot scale of two spiral wound RO membrane (5 m²) in series to treat wastewater containing copper from the first rinse of a copper sulphate (blue copper ion) electroplating line at a factory in Hong Kong. The feed copper concentration was 340 ppm while the treated water contained only 4 ppm. This readily met the Hong Kong government requirements for discharge of the wastewater. The study also confirmed the possibility of reducing copper concentration in the treated water by increasing the applied pressure at any temperature. Moreover, permeate flux increased due to increasing transmembrane pressure or applied temperature. However, the temperature had an insignificant impact on permeate concentration.

Xijun et al. (1997) tested the efficiency of a treatment system consisting of two spiral wound non-cellulose composite membranes in series with a total membrane area of 10 m² type ATFRO (APV, Denmark) to treat the wastewater of an electroplating plant containing copper. A pretreatment step of UF membrane was added to mitigate the fouling propensity of RO membranes. The results confirmed that the RO membranes could remove around 96.4% of copper. A laboratory-scale RO containing composite spiral wound membrane (RE2012-100) of 1.95 m² area was tested by Mohsen-Nia et al. (2007) to remove copper and nickel from a mixed salt system. They reported a maximum rejection of 98% for copper and nickel with a somewhat higher rejection of copper due to its larger size.

Cséfalvay et al. (2009) investigated the performance of a bench-scale crossflow membrane filtration apparatus of a flat sheet RO membrane (28 cm²) to remove copper-sulphate and copper-nitrate solutions as model wastewaters at 25 °C. The copper-sulphate rejections of the RO membranes were found to be more than 95%.

4.4.3.6 Iron

Iron is specifically found in different concentrations in surface water and groundwater, and in wastewater streams from steel production, which consumes a significant amount of water. For instance, the iron and steel industry of China consume around 14% of the total industrial water used in China (Huang et al., 2011). More importantly, a low concentration of iron can impair water distribution systems due to its

link to aesthetic and operational issues, including colour, staining, and deposition. This is why physical, chemical, and biological treatment methods have been commonly used to remove iron from various wastewaters under given process conditions (Ellis et al., 2000; Sharma et al., 2001).

Huang et al. (2011) investigated the feasibility and effectiveness of a constructed wetland (CW) as a pretreatment method in a hybrid process consisting of UF and RO (CW/UF/RO) to remove iron and manganese from the wastewater of Baosteel Co. Ltd. (China). The results displayed a significant reduction of iron and manganese concentrations in the effluent from the constructed wetland to around 0.05 mg/L and 0.04 mg/L, which corresponds to 96.9% and 92.5% removal of iron and manganese, respectively.

Talalaj (2015) evaluated the performance of a disc tube RO thin-film composite polyamide membrane (9 m²) for the removal of different organic and inorganic compounds, including iron, from leachate collected from a municipal landfill in the north-eastern part of Poland. The landfill typically includes 0%–95% of inorganic material and 5%–20% of organic compounds (öman and Junestedt, 2008). The RO treatment process was confirmed to be a feasible process for all parameters analysed in leachate. In this respect, the mean feed concentration of iron was 5.2 ppm and the removal efficiency was high at 97.6%.

4.4.3.7 Lead

Lead is a potential toxic heavy grey metal (insoluble in water) that can be extensively released into the environment from the wastewater of mining, metal plating, tannery, radiator, alloy, and battery industries (Acharya et al., 2009). The high level of heavy metals and especially lead in local water streams is a clear threat to public health even at very small concentrations. Lead (non-degradable) has been strictly limited to be released into the water system by the US Environmental Protection Agency in 2003 to 0.006 ppm as the MCL standards (Babel and Kurniawan, 2004). However, the US EPA and WHO have limited lead in wastewater and drinking water to 0.05 ppm (Ucun et al., 2003; Goel et al., 2005). Therefore, lead can be considered as a key priority for removal due to its high solubility in aquatic environments, which would endanger public health and can cause brain disorder and death (Mondal, 2009; Singha and Das, 2012). There are several conventional treatment methods for removing lead from wastewater. They include precipitation, ion exchange, liquid-liquid extraction, adsorption, and membrane technology (Gherasim et al., 2013; Gherasim and Mikulášek, 2014).

The cost-effective precipitation treatment method has been extensively used to remove lead ions up to ppm levels from water. However, this reduction is not satisfactory based on the requirements of water quality standards (Abdel-Halim et al., 2003). Furthermore, a low pH medium can passively affect the performance of precipitation in addition to generating a sludge with high water content (Arbabi et al., 2015). Similarly, ion exchange is a relatively expensive treatment method to remove lead ions. This method is not efficient for high-concentration solutions due to the organic fouling problem on the matrix in addition to its high sensitivity to pH (Ahluwalia and Goyal, 2007). Membrane technology and specifically the RO process have been found to provide a cheaper and more effective technology for recovering a wide

range of heavy metals, including lead ions, from industrial wastes (Gherasim and Mikulášek, 2014; Thaçi and Gashi, 2019). However, membrane fouling and its high sensitivity to operating conditions are highlighted as the main disadvantages (Akpör and Muchie, 2010) of the RO process.

Algureiri and Abdulmajeed (2016) tested the performance of spiral wound RO process (7.9 m² of effective area, FilmTec membrane) to remove several heavy metals including lead from synthetic industrial wastewater at different feed concentrations. This provided a promising solution for efficiently removing lead at around 97.5%, with a corresponding removal of 98.5%, 96% nickel and copper, respectively. Interestingly, the experiments confirmed the possibility of reclaiming and reuse of the wastewater due to low levels of heavy metals.

4.4.3.8 Nickel

Nickel is a toxic non-biodegradable heavy metal that can exist in the effluents of wastewater of many industries including printing, electroplating, alloy, steel production and battery manufacturing (Yang et al., 2009; Mobasherpour et al., 2012). It is therefore important to remove it from wastewater before it gets discharged into surface waters or reused even at low concentrations (Rohini et al., 2014). The threshold of nickel in wastewater is set at 2 ppm by the legal Hungarian law (Borbély and Nagy, 2009). Whereas, this is restricted to 0.2 ppm the US EPA in 2003 (Babel and Kurniawan, 2004). Several essential treatment methods have been used to remove nickel from wastewaters including chemical precipitation, activated carbon adsorption, ion exchange, chemical reduction, flocculation, filtration, evaporation, solvent extraction, biosorption, RO and electrodialysis (Dhokpande et al., 2013) in addition to RO process.

Qin et al. (2002) investigated the performance of crossflow recirculated mode of three RO flat sheet composite membranes in series to treat the spent rinse water from a nickel-plating factory in Singapore and then reuse it as alkaline rinse water. The impact of feed concentration and pressure and including UF pretreatment process on the process performance were examined at 25 °C and 0.25 m/s of temperature and feed velocity, respectively. This experimental work confirmed the rejection of nickel and nitrate at 99.8% and 95%, respectively. It was also reported that a UF membrane prior to RO membrane could reduce the fouling propensity by 30%–50%.

Ipek (2005) experimentally investigated the performance of a combined pretreatment filtration and RO process in a pilot-scale plant to remove nickel and zinc from wastewater. This indicated high removal of nickel and zinc around 99.2% and 98.8%, respectively. An insignificant impact of inlet feed concentration on the ion removal was noticed.

Rodrigues Pires da Silva et al. (2016) focussed on removing heavy metal ions of nickel and copper (pure and in a mixture) from a highly diluted wastewater using low-pressure polyamide-urea advanced composite RO membrane type 4040-X201-TSA (produced by the Trisep Corporation). The RO system worked in batch mode where the mixtures of nickel and copper were always prepared in a stoichiometric ratio. Also, ethylenediaminetetraacetic acid (EDTA) was used as a chelating agent for aqueous solutions. The experimental work confirmed around 99.0% removal of nickel and copper ions. Moreover, the use of EDTA reduced the concentration of

pollutants in the permeate side due to forming larger size of the complex compared to the ion in the aqueous phase.

Al-Alawy and Salih (2017) studied the efficiency of a pilot-scale RO process of a spiral wound module containing a polyamide membrane to retain several inorganic heavy metals including nickel from synthetic electroplating wastewater. The experiments showed an excellent removal efficiency of 99.49% together with a high removal of around 99% for zinc, copper, and chromium in line with the permissible limits of disposing wastewater.

4.4.3.9 Mercury

Mercury was assigned as one of the 13 metals by the US EPA's priority pollutants, with a strict restriction of 1.4 µg/L (in 1997) and 0.00003 ppm (in 2003), respectively, as its MCL standards (Babel and Kurniawan, 2004; U.S. Environmental Protection Agency, 2011). The stricter emission standard is due to its high toxicity and widespread existence in several industrial applications and various types of laboratory equipment and instruments such as refineries, coal-fired power plants, electrodes, batteries, thermometers, barometers, manometers, and mining (Parham et al., 2012). Several treatment technologies have been used to remove mercury from wastewater. These include the use of precipitation, coagulation/co-precipitation, activated carbon adsorption, ion exchange treatment, chemical reduction, and membrane technology. Also, several studies were conducted using different membrane processes, such as ultrafiltration, charged filtration, crossflow microfiltration, and RO process (Ebadian, 2001).

Urgun-Demirtas et al. (2012) investigated the ability of a bench-scale of several membrane types including an RO membrane to treat an oil refinery effluent and achieve the stringent limit of mercury of less than 1.3 ng/L in the surface water discharge (Water quality guidance for the great lakes system, 1995) at lower pressures of 20.7 bar.

4.4.3.10 Nitrogenous Compounds

Nitrogenous compounds can cause serious health disorders when discharged into the surrounding water (Qin et al., 2005b). These compounds can disrupt aquatic ecosystems in a severe way. A number of practical treatment methods have been adopted for the removal of nitrogenous compounds from wastewater with inconsistent degrees of success and with high energy consumption and the production of secondary high-toxic by-products (Mook et al., 2012).

The feasibility of a single of RO process in combination with other technologies to remove nitrogenous compounds from wastewater is highlighted in some examples, as shown in the next section.

Schoeman and Steyn (2003) confirmed the feasibility of applying an RO process for water denitrification and water desalination in a rural area. This showed a high-efficiency of removing nitrate nitrogen and TDS. Specifically, the feed concentration of nitrate nitrogen and TDS were decreased from 42.5 ppm to 0.9 ppm and from 1292 ppm to 24 ppm in the permeate, respectively, at 50% water recovery.

Qin et al. (2005a) applied a wind-driven spiral wound RO membrane (7.6 m²) to remove the major contaminants of nitrogenous compounds (ammonia, nitrite, and

nitrate) from aquaculture industry wastewater. The RO membrane achieved 90% to 97% of nitrogen removal with 39%–57% of wastewater recovery rate.

The technical feasibility of a prototype wind-driven RO system was used by Qin et al. (2005a) to reject nitrogenous wastes from aqua-cultural wastewater. Basically, the wind energy is converted into hydraulic pressure for the RO process by using a multi-blade windmill. This involved the use of a spiral wound thin-film composite membrane (7.6 m²) type FilmTec XLE-4040 manufactured by Applied Membranes Inc. (Vista, CA). The treatment system guaranteed a 90% to 97% removal rate of nitrogen with water recovery of 40%–56%. Moreover, no more than 0.04 mg/L of ammonia concentration was detected in the reclaimed water. Interestingly, the chemical analysis affirmed zero concentration for nitrite and nitrate. This process yielded high-quality water, which can be reused in different applications. A specific advantage of renewable energy source was used to reduce the fossil fuel-based energy consumption of the RO process.

Madaeni and Koocheki (2006) employed a pilot plant of two spiral wound RO membranes type FilmTec TW30HP-4641 (11.89 m²) in a series configuration to treat wastewater containing nitrogenous compounds of nitrate, nitrite, sulphite, and phosphate. The influence of operating pressure, temperature, and feed concentration on the process rejections was investigated. They observed that both feed temperature and transmembrane pressure had a positive impact on permeate flux, while the feed concentration had the most impact on the removal of nitrate, nitrite, sulphite, and phosphate. More importantly, the experiments generated an average rejection of around 96%. However, a complete rejection of 100% of the tested compounds was obtained at optimised operating conditions. The same crossflow filtration system was used by Madaeni and Koocheki (2010) to remove the same compounds where the removal of nitrite and nitrate ions could be enhanced to reach 99% by adding monopotassium phosphate (KH₂PO₄) into the solution.

Jadhao and Dawande (2012) tested the potential of a laboratory-scale batch operation of a combined process of two modules—spiral wound polyamide RO membrane and cellulose acetate UF membrane—to remove total nitrogen (TN), ammonia nitrogen (NH₄), and nitrate nitrogen (NO₃) from hospital wastewater. This study also included the investigation of the chemical oxygen demand (COD), biochemical oxygen demand (BOD), total phosphorus (TP), and suspended and dissolved solids. The results proved the superior performance of the RO process, where 90%, 98%, and 96% of TN, NH₄, and NO₃, respectively, were removed. Occasionally, the experiments also showed that the RO process could totally remove TDS and TSS.

Chon et al. (2014) evaluated the performance of a pilot plant hybrid system of a coagulation–disk filtration (CC–DF) process and the dual membrane process of microfiltration and RO membranes to remove organic materials, metals, metalloids, nitrogen, and phosphorous pollutants from the secondary effluents of the Ansan wastewater treatment plant (Ansan, Gyeonggi-do, Korea). The result indicated a higher efficiency of the RO membrane to reject most of the water pollutants, including nitrogen compounds, than the other treatment methods. More specifically, nitrate ions were not efficiently removed by the CC–DF and MF membranes, but were totally resolved by RO membranes by removing more than 86% of nitrate from

the permeate of the MF membrane. This is attributed to the impact of two combined mechanisms of separation: size exclusion and charge repulsion of RO membranes. However, the removal of boron was not satisfied because of its non-ionised form at the neutral pH (i.e. boric acids).

Talalaj (2015) evaluated the effectiveness of rejecting organic and inorganic pollutants from landfill leachate using the RO process. Leachate is usually characterised by a high concentration of ammonia and other pollutants such as chlorides, iron, and sulphates. The RO process was found to be an adequate treatment method for all the tested parameters in leachate. This included the removal efficiency of 98.7% and 99% for ammonia nitrogen (N-NH_4) and total inorganic nitrogen, respectively. Also, 97%, 97.2%, 93%, 97.6%, and 98% of chemical oxygen demand, electroconductivity, cyanides (CN), iron (Fe), and chlorides (Cl), respectively, were removed. However, only 83%, and 86% removal for sulphates (SO_4) and sulphide (S), respectively, were achieved.

4.4.3.11 Highly Toxic Organic Compounds

This section specifically illustrates the performance of an RO process to remove highly toxic organic compounds from wastewater.

4.4.3.11.1 Phenol and Phenolic Compounds

Sundaramoorthy et al. (2011) and Srinivasan et al. (2011) investigated the efficiency of eliminating chlorophenol and dimethylphenol from wastewater using a pilot-scale RO process using single spiral wound module and confirmed 83% and 97% rejection, respectively. This was obtained using 13.58 atm, $2.583\text{E-}4 \text{ m}^3/\text{s}$, and 31°C of feed pressure, flow rate, and temperature, respectively. Also, this was associated with 22% and $2.034 \text{ kWh}/\text{m}^3$ of total water recovery and energy consumption, respectively. The relatively low chlorophenol removal was probably due to its high hydrophobicity properties in water (slightly dissolved in water) (20 g/L at 20°C) besides its high activity because of the existence of hydroxyl group, which accelerates its penetration through the membrane texture. Srinivasan et al. (2010) presented the phenol rejection between 64% and 87% using the same experimental apparatus of the RO process.

Several types of NF nanofiltration and RO flat sheet membranes (0.072 m^2) of plate and frame module were examined by Li et al. (2010) to eliminate phenol from wastewater at a wide range of operating conditions. The phenol removal of RO membrane type (RO99) was found to be between 76% and 86% at feed pressure and varying between 4.9 and 29.6 atm and fixed feed concentration, velocity, and temperature of 500 ppm, 0.58 m/s and 25°C , respectively.

Arsuaga et al. (2011) carried out a set of experiments and confirmed that commercial flat sheet RO membrane types TFC-HR and BW-30 (139 cm^2) were able to reject 75% of phenol. Tabassi et al. (2014) explored the efficiency of a pilot plant of a single commercial polyamide thin-film composite spiral wound RO membrane type SG 2514TF (GE Osmonics) of 0.6 m^2 in eliminating phenol from synthetic aqueous solutions of different concentrations. The impact of several operating conditions was studied on the process performance, and the optimum rejection achieved exceeded 80%.

A crossflow filtration system of a low-pressure polyamide thin-film composite spiral wound RO membrane type TW30–1812–100 (0.446 m²) was used by Khazaali et al. (2014) to achieve an optimum bisphenol A (BPA) removal from wastewater. The study affirmed the value of 87% removal at optimum operating pressure.

The aforementioned literature demonstrates that phenol and phenolic derivatives were not rejected completely by RO membranes.

4.4.3.11.2 *N*-nitrosamine Compounds

The efficiency of the RO process specifically for *N*-nitrosamine and more importantly for NDMA (N-nitrosodimethylamine-D6) (C₂H₆N₂O) removal continues to be a challenge as demonstrated by a brief state-of-the-art review in the next section.

Steinle-Darling et al. (2007) used a flat sheet of three commercial RO membranes to test the removal of seven *N*-nitrosoalkylamines from wastewater. They found that NDMA rejection was limited to 54%–70%. However, Plumlee et al. (2008) and Krauss et al. (2010) confirmed the range of 24% to 56% and 40% to 70%, respectively, as the efficiency of the RO process to remove NDMA. The different membrane types can be attributed to different efficiencies of NDMA removal.

Fujioka et al. (2012) and Fujioka et al. (2013) employed a laboratory-scale system of low-pressure NF/RO membranes to explore the removal of eight compounds of *N*-nitrosamine from wastewater. This confirmed a range of 8%–80% for the removal of NDMA under the same operating conditions, which is also based on the membrane type. A full-scale spiral wound RO membrane filtration system was used by Fujioka et al. (2014) to investigate its efficiency for the rejection of *N*-nitrosamine. This time, three and seven pressure vessels (PV) connected in series were used, where each PV held one membrane of 7.9 m² as an effective area. The NDMA removal varied between 40% to 61% and 49% to 35% for the three and seven PV, respectively. Moreover, an optimum value of rejection of eight *N*-nitrosamine compounds between 62% and 99% was observed using 10.1 atm pressure, 2.43E-3 m³/s, and 20 °C, of operating pressure, feed flow rate, and temperature, respectively. The uncharged and quite hydrophilic properties of NDMA cause a repulsion of these molecules as they do not stick to the membrane and absorb poorly where it stays in the water because of their high hydrophilicity³ (log *K*_{ow} = −0.57) (highly dissolved in water, water solubility: 290 g/L at 20 °C) (Schäfer et al., 2010). The low charge measurement of NDMA (*pK*_a) (acid dissociation constant) of less than one causes a lower rejection in RO membranes at ambient pH (pH region of 6–12) (Lee et al., 2008). Also, another explanation of low rejection of NDMA can be drawn from the smaller molecular size compared to membrane pore size. Basically, any solute having a smaller size than the molecular weight cut-off⁴ of the membrane would be poorly rejected. Note, NDMA (MW 74.1) has a size of 73 Da (daltons) while MWCO has a size of 100 Da (Andrea et al., 2010). It is therefore fair to say that the solute properties of NDMA including its molecular weight (size exclusion), high hydrophilicity, and low charge solute are possibly the main reasons of its low removal rate in RO membranes. This means that there is room for improvement in so far as the removal of NDMA using a laboratory-scale and full-scale RO wastewater treatment process. In summary, whilst RO membranes have been shown to provide a promising solution, their efficiency for eliminating NDMA is yet to be proven.

4.5 CONCLUSIONS

RO technology was initially developed for the desalination of seawater and brackish water to produce drinking water. However, its rapid growth in various applications has rendered RO a commercially attractive separation process for the treatment of industrial effluents. Undoubtedly, the membrane technology and especially the RO process are now recognised as a promising technology for water recycling and reuse. The use of RO yields a low level of the pollutant concentration in the permeate, which in turn accelerates the reclamation of good-quality water for yet more applications. Additionally, it can be considered as the cheapest treatment method compared to conventional processes.

This chapter has reviewed and discussed the feasibility of the RO process for the removal of several organic and inorganic pollutants, including the highly toxic phenolic and N-nitrosamine compounds from wastewater. It is clear from the research presented in this chapter that RO remains as the most promising and economically viable separation process for removing harmful contents from wastewater at levels commensurate with environmental legislation. The state of the art provided in this chapter indicates that significant progress has been made for removing a wide range of hazardous chemicals and micropollutants from wastewater, but there is still room for improvement for achieving a better and cheaper solution.

It is evident, therefore, that membrane separation technology is increasingly being approved in several industries due to its ability to remove highly toxic substances from several industrial wastewaters. However, this technology still has some key challenges relating to the removal of highly toxic organic compounds such as phenolic and N-nitrosamine compounds. There is therefore an urgent need to develop a new treatment process specifically for removing N-nitrosamine precursors found in water treatment plants. Such a process must explore alternative polymers to enable high-performance membranes to eliminate these harmful compounds.

NOTES

- 1 COD is an indicative measure of the amount of oxygen that can be consumed by reactions in a measured solution, which is expressed in mass of oxygen consumed over volume of solution (mg/l). Therefore, COD can be used to quantify the amount of organics in water.
- 2 MWCO is defined as a general guide for the separation ability of a membrane to remove 90% of a species based on its molecular weight (Rohani et al., 2011).
- 3 A hydrophilic molecule is one whose interactions and affinity with water and other polar substances are more thermodynamically favourable than their interactions with oil or other hydrophobic solvents. They are typically charge-polarized and capable of hydrogen bonding. This makes these molecules soluble not only in water but also in other polar solvents (Merriam-Webster dictionary).
- 4 MWCO is defined as the molar mass above which more than 90% of a given compound is rejected (Andrea et al., 2010).

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5 Modelling and Model Validation of Reverse Osmosis Process for Wastewater Treatment

5.1 INTRODUCTION

The reverse osmosis (RO) process has been used to treat sea and brackish water as well as industrial effluents. Its use has also been extended to different types of industrial applications including the textile, paper, electrochemical, and biochemical industries. This has demonstrated that an RO process can indeed provide an effective and economical treatment process in a growing separation market.

The spiral wound concept is the most commonly used model in RO due to its amenability for use in a variety of different applications. However, there remains the challenge of having a reliable design, which will yield a high process performance. There is therefore an important need to develop accurate mathematical process models, which would facilitate the evaluation of alternative process designs and operations without requiring expensive experimental or pilot studies. Such evaluation can be benchmarked against a number of performance measures including maximum rejection of pollutants, maximum profit, minimum operating cost, and minimum energy consumption.

Modelling of any process requires a full understanding of the underlying process mechanism, which includes several independent variables (inputs) and dependent variables (outputs) expressed in mathematical relationships. Any model developed can be characterised as black box, grey box, or white box depending on how much of the underlying physics of the process are known. Figure 5.1 briefly defines each of these types of process models.

The white box or first principle-based models for complex processes such as spiral wound RO process usually consists of a set of non-linear partial differential and algebraic equations (PDAEs) which can be used to predict and optimise the process behaviour. Several such mathematical models appear in the literature, and they are used to predict the transport phenomena in the RO process, particularly those that accurately relate to the removal of organic and non-organic compounds from wastewater.

These models are often based on the solution-diffusion model and the irreversible thermodynamic model to express the transport of the solvent and solute through the membrane. They are the only two models referred to widely in the literature. The

Different Types of Process Models*Black Box Models*

- Only interested in input-output mapping
- Underlying physics not known
- Not suitable for capturing process dynamics
- Computationally less expensive
- Unreliable when conditions change, may need tuning
- Suitable for steady state processes and to some extent unsteady processes (limited)

Example: neural network-based models described in terms of input-output (Mujtaba and Hussain, 2001; Tanvir and Mujtaba, 2006)

Grey Box Models

- Underlying physics partially known
- More reliable than black box model
- More computationally expensive than black box model
- Can capture process dynamics to some extent and therefore may be suitable for control studies

Example: hybrid process model (in between black box and white box models). Part of the model is based on input-output mapping (Mujtaba et al., 2006).

White Box Models

- Underlying physics known
- Computationally very expensive
- Reliable prediction of process dynamics
- Suitable for control studies

Example: processes described by mass balance, energy balance, thermodynamics, chemical reactions, geometry, etc.

Often known as first principle-based models (Al-Obaidi and co-workers, 2016–2019)

FIGURE 5.1 Different types of process models (Mujtaba, 2017, 2019).

simple concepts of these models have led to them being used extensively in many applications. However, the majority of these models rely on approximate calculations based on average conditions of the membrane sides without considering the variation of operating parameters along the membrane dimensions (analytical models). In other words, these models do not consider the impact of operating parameter variation along the membrane dimensions. Only a few models have been recently

developed to assess the variation of operating parameters along one and two dimensions of the membrane. The development of distributed models is based on a thorough understanding of the flow pattern inside the module for enhancing the process design. Specifically, the merit of distributed modelling is the consideration of the variances of all the operating parameters, the pattern of feed flow rate, solvent and solute fluxes, and mass transfer coefficient along the axial and tangential axes of the feed and permeate sides. This offers a more accurate prediction of the performance of the process in comparison to lumped models.

It is important to note that a two-dimensional modelling system has the advantage of providing a facility for predicting process performance more accurately than that of one-dimensional modelling. This is because the pattern of feed flow rate along the tangential direction for both the retentate and permeate sides are taken into consideration.

One of the requirements for designing control systems of an RO process is the development of a dynamic model, which can predict the transient characteristics of the plant. It can also be argued that the dynamic modelling can yield other advantages compared to steady state modelling. The dynamic model includes the time parameter, which allows the modelling of the behaviour of the process against the operational time. It is therefore highly advantageous to have a dynamical model capable of yielding a more efficient process control strategy and maintaining the separation cost at an acceptable level.

This chapter reviews the conceptual modelling and membrane transport theories of the RO process and will explore the remaining modelling challenges. In line with this, this chapter focusses on presenting all the available models and associated performances of wastewater treatment methods based on the spiral wound RO process for the removal of highly toxic compounds from wastewater. In other words, this chapter looks into the evolution of the models developed (lumped and distributed steady state and dynamic) in the last decade for a spiral wound RO process for the removal of organic compounds from wastewater. Also, this chapter highlights the scope and limitations of the transport models based on the irreversible thermodynamics and the solution-diffusion models previously used by several researchers. These models can be used to simulate the phenomenon of solvent and solute transport through the membrane. This phenomenon incorporates the fluid physical properties required for predicting the rejection of organic compounds for a single-stage RO process with spiral wound membrane module and multi-stage RO process. Finally, this chapter provides a comprehensive analysis of various lumped and distributed models validated against experimental results gathered from the literature.

5.2 MODELLING RATIONALE

The modelling of any industrial process helps clarify an understanding of the process mechanism. This can then be used to design a suitable pilot or full-scale process and evaluate the impact of the design and operating parameters on the process performance using sensitivity analysis and simulation. The modelling can also help improve process performance via optimisation. However, before a model can be used

confidently for any purpose (simulation, optimisation, control, design), it must be validated against experimental or plant data first.

5.3 RO PROCESS MODELLING CHALLENGES

There are several challenges in process modelling, including an accurate apprehension of the process mechanism and laborious appraisal of different designs via simulation and optimisation. More specifically, the modelling of complicated processes, such as wastewater treatment RO process due to a wide range of compounds with different transport mechanisms involved in the process, is far from trivial. Generally, there are two types of models: steady state and dynamic.

Steady state models employ constant flows and loads in respect to time compared to dynamic models, which use variable flow and loads. In other words, the inclusion of time variation in the dynamic model, compared with zero-time derivation in steady state models, is the main difference between these two models. It is therefore fair to say that the development of any dynamic model can add further complexity compared to the steady state model.

Providing an accurate dynamic model is an important task, which should implicitly predict the process performance indicators compared to steady state models. Dynamic models are useful for accurately assessing the response of the process during the process operation.

The concentration polarisation and fouling issue are considered the biggest drawbacks of the RO process. These can significantly deteriorate the water permeation through the membrane, which means that the filtration process must be stopped periodically to carry out back flashing in order to restore the process performance. A multi-stage parallel RO process with optimally scheduled cleaning in place, however, can potentially avoid the complete shutdown of the process (Sassi and Mujtaba, 2013).

5.4 MEMBRANE TRANSPORT THEORIES

Several RO theoretical transport models have been explored by various researchers to predict solute and solvent fluxes resulting in three types of models: the pore model (diffusion- and convection-based), the non-porous model (diffusion-based), and the phenomenological model based on thermodynamics (Soltanieh and Gill, 1981). However, a thorough literature review carried out by Al-Obaidi et al. (2017a) indicated that the irreversible thermodynamic model and solution-diffusion model are the most widely used models to describe the membrane transport mechanism. The next section highlights in detail these important models and explains separation phenomena of water and solute in RO process.

5.4.1 SOLUTION-DIFFUSION MODEL

The solution-diffusion model can be considered as one of the simplest non-porous or homogeneous models related to transport mechanism criteria. Lonsdale et al. (1965) first proposed this model emphasising that the separation process can be achieved

in RO units by both dissolving and diffusing each species in the solution (salt and solvent) independently through the membrane, without considering the interaction between salt, solvent, and membrane. The assumption here is that each solvent and solute is dissolved in the membrane independently on the high-pressure side. They are then diffused in individual fluxes through the membrane under the impact of pressure and concentration differences. The quality of permeate separation occurs due to the mobility of dissolved solute and the rate of its diffusion (Wijmans and Baker, 1995). Thus, the fluxes of solvent and solutes are effectively dependent on the values of solubility and diffusivity of solvent and each solute in the membrane (Lonsdale et al., 1965; Jonsson, 1980).

In line with this model, the solvent flux J_w (m/s) is proportional to the divergence between the hydraulic pressure difference ΔP_b (atm) and the osmotic pressure difference $\Delta \pi$ (atm) across the membrane by the construction (Lonsdale et al., 1965).

$$J_w = A_w (\Delta P_b - \Delta \pi) \quad (5.1)$$

$$\Delta \pi = RT_b (C_w - C_p) \quad (5.2)$$

A_w (m/s atm) is the water permeability constant, ΔP_b (atm) is the transmembrane pressure, and $\Delta \pi$ (atm) is the osmotic pressure difference along the length of the membrane L (m). $(\Delta P_b - \Delta \pi)$ is the quantity of force per unit area required to cope with the osmotic pressure and to release pure water from the feed solution. C_w and C_p (kmol/m³) are the solute concentration at the membrane wall and permeate side, respectively. R and T_b (0.082 (atm m³/K kmol), K) are the gas law constant and operating temperature, respectively. Also, the salt flux J_s (kmol/m² s) is formulated as:

$$J_s = B_s [C_w - C_p] \quad (5.3)$$

B_s is the solute transport parameter of the membrane. Lonsdale et al. (1965) stated that the membrane solvent water permeability constant depends on the structure of the membrane, while the salt permeability constant depends on salt composition and membrane structure. It is easy to see that this model assumes that the salt flux does not depend on the pressure difference. Occasionally, the solution-diffusion model requires only a few parameters to measure the mechanism of transport including the water and solute transport parameters. Finally, one of the imperfections of this model is that it neglects the impact of pressure on solute flux, the inclusion of pore flow, and the membrane characteristics.

5.4.2 IRREVERSIBLE THERMODYNAMIC MODEL

The concept behind the irreversible thermodynamic model is derived from the principle theory of non-equilibrium thermodynamic systems, which is a type of thermodynamic that simulates most systems found in nature, such as the transport processes (Fowler and Guggenheim, 1965). Basically, the irreversible thermodynamic model depends on non-equilibrium thermodynamic equations, which consider the membrane as a black box where slow processes are occurring near the equilibrium.

Unfortunately, this implies that there is insufficient information for describing flow, transport mechanism, and the structure of the membrane. The latter can be accounted for as one of the imperfections of the model, which means the applicability of using the irreversible thermodynamic model for accurate speculation of membrane separation cannot hold.

The starting fundamental formula for the irreversible thermodynamic model was established by Kedem and Katchalsky (1958) and then by Spiegler and Kedem (1966) for a dilute two-component non-electrolyte system of water and solute as linear and non-linear equations respectively relating to the fluxes of these components. Interestingly, they found that these equations, which are assumed in the solution-diffusion model, have only two permeability coefficients—the solute permeability coefficient and the water permeability coefficient, which were judged unsuitable for the irreversible thermodynamic processes. They believed that there should be a combination of three rather than two parameters. Therefore, a third parameter of the reflection coefficient has been added to express the broad criteria of a sensible interaction between the solute-solvent-membrane, which generates and enhances an acting force between them. It is believed that the interaction between the solute, solvent, and membrane are included in this model for the first time, and that the phenomenological relations can explain the fluxes better (Van Gauwbergen and Baeyens, 1998; Jonsson, 1980; Sapienza et al., 1990). These assumed that the variation of pressure and concentration gradients (the chemical potential) to be linear with low levels of solvent flow rates and the three membrane parameters—specific hydraulic permeability, local solute permeability, and reflection coefficient—are constant. Moreover, the reflection coefficient can be considered as a scalar of the membrane semi-permeability, by varying from zero for non-ideal membrane of non-solute selectivity to one of the ideal membranes, which passes only solvents (Spiegler and Kedem, 1966). Hence, the transport models have been modified further to include the reflection coefficient parameter, which describes the solute rejection. This is used as a parameter to evaluate the selectivity of solutes by the membrane (Zelman, 1972; Muldowney and Punzi, 1988) and measure the coupling of solute-solvent fluxes through the membrane (Marriott, 2001). Therefore, the water and solute flux equations for a single solute system are:

$$J_w = L_p (\Delta P_b - \sigma \Delta \pi) \quad (5.4)$$

$$J_s = \omega RT (C_w - C_p) + C_b^- (1 - \sigma) J_w \quad (5.5)$$

L_p (m/atm s) and σ (–) are the specific hydraulic permeability of the membrane and reflection coefficient, respectively. σ equals 0 for complete coupling between the solvent and solute fluxes within the membrane and 1 if no coupling exists (solution-diffusion model). ω (kmol/m² s atm) C_b^- (kmol/m³) are the local solute permeability and average solute concentration that can be defined as:

$$C_b^- = \frac{C_b - C_p}{\ln \left(\frac{C_b}{C_p} \right)} \approx \frac{C_b + C_p}{2} \quad (5.6)$$

C_b (kmol/m³) is the bulk concentration at the feed channel. Eq. (5.4) shows that the reflection coefficient controls the osmotic pressure. However, Eq. (5.5) expresses the solute flux by incorporating of two terms, the first of which illustrates the diffusive solute flux, while the second term illustrates the solute transport mechanism by convection, which is caused by the coupling between the solute and solvent through three parameters. In the case where there is no coupling between the solvent and solute, the convection term will be 0 (solution-diffusion model).

Unfortunately, the expression of average concentration (Eq. 5.6) is not exact in the event of a high solvent flux or high concentration difference (Mason and Lonsdale, 1990). Furthermore, the three transport parameters of this model are independent of each other and can simply represent the original phenomenological coefficients. They can be expressed as less independent of concentration (Kedem and Katchalsky, 1958; Jonsson, 1980; Soltanieh and Gill, 1981; Van Gauwbergen and Baeyens, 1998).

The main difference between the irreversible thermodynamic model and solution-diffusion model is that the interaction between the solute, solvent, and membrane are specifically included in the irreversible thermodynamic model. As a result, this model is more widely used to describe the performance of the membrane separation in RO systems than any other investigated models (Mason and Lonsdale, 1990; Murthy and Gupta, 1998). Mujtaba (2012) has shown, however, that the solution-diffusion model is the simplest non-porous or homogeneous model and one that is widely used in RO systems.

5.5 OVERVIEW OF RO PROCESS MODELLING FOR SEAWATER AND BRACKISH WATER DESALINATION

In the past two decades, many models have been developed relying on different assumptions for a spiral wound RO process for the removal of total dissolved salts from aqueous solutions. These models have been applied to seawater and brackish water desalination and validated against experimental data.

A lumped model was developed by Gupta (1985) for a spiral wound module under laminar and turbulent flows and based on the solution-diffusion model. However, it presumes constant mass transfer coefficient and solute concentration at the feed channel and neglects solute concentration at the permeate channel. Avlonitis et al. (1991), Boudinar et al. (1992), Avlonitis et al. (1993), and Avlonitis et al. (2007) presented two-dimensional (2D) (x and y) steady state models based on the solution-diffusion principle. These models considered a full axial flow of solution, but they neglected the components of the tangential feed flow and axial permeate flow. Also, they assumed constant physical properties, ignoring the variance of permeate concentration and overlooking the concentration polarisation impact. Moreover, Boudinar et al. (1992) stated that the pressure loss in the two channels was a function of feed and permeate friction parameters (Darcy's law for porous media).

Marriott and Sørensen (2003) developed a 2D dynamic model for a spiral wound RO module by using mass, momentum, and energy balance equations. Whilst this model has relaxed several common assumptions, the variation of bulk concentration due to solvent flux through the membrane was not considered. Geraldès et al. (2005) developed a one-dimensional (1D) steady state model for spiral wound RO

membranes based on the solution-diffusion model by ignoring the pressure drop in the permeate channel and also the diffusion flow in the feed channel.

Based on the three-parameter model of Spiegler and Kedem (1966), Senthilmurugan et al. (2005) and Mane et al. (2009) developed models for turbulent flow by considering the pressure drop in both channels. Also, Mane et al. (2009) used the irreversible thermodynamic principles to develop a 2D model for the feed flow rate and stimulated the rejection of boron by using two commercially spiral wound modules in pilot-scale and full-scale RO seawater desalination processes with varying pH and pressures.

Oh et al. (2009) developed a comprehensive lumped model based on the solution-diffusion principles for the simulation and optimisation of spiral wound RO system for seawater desalination. They assumed constant mass transfer coefficient, constant water flux, and constant permeate pressure. Kaghazchi et al. (2010) proposed a 1D model based on the solution-diffusion model where the bulk flow rate was calculated as an average value of inlet and outlet feed flow rates.

For an industrial scale RO desalination process, Chen-Jen et al. (2010) studied the dynamic characteristics and process operation by developing a mathematical one-dimensional dynamic model. This work combined the model of Oh et al. (2009) with that of Marriott and Sørensen (2003) and considered the impact of solvent flux on the concentration. Patroklou et al. (2013) developed a model for boron rejection based on the irreversible thermodynamic model and validated the model using the experimental data of Mane et al. (2009).

Generally, all the models were developed for a spiral wound RO process and validated against experimental data derived for sea and brackish water (Sundaramoorthy et al., 2011a).

5.6 OVERVIEW OF RO PROCESS MODELLING FOR WASTEWATER TREATMENT

State-of-the-art successful models developed for RO processes, specifically for spiral wound modules for the removal of organic compounds from wastewater and validated against actual wastewater treatment experiments, are illustrated in this section.

Al-Bastaki (2004) investigated a lumped parameter model to assess the transport phenomena of a spiral wound RO process used to remove Na_2SO_4 salt and methyl orange dye ($\text{C}_{14}\text{H}_{14}\text{N}_3\text{NaO}_3\text{S}$) from wastewater. The model was developed based on a solution-diffusion model considering the concentration polarisation of both dye and salt. The model was validated against experimental results and agreed well with general trends at low operating pressures. However, the model could not predict the process performance at high pressures.

Ahmad et al. (2007) developed a lumped parameter model suitable for any multiple solutes system for dynamic simulation and prediction of membrane filtration in terms of permeate flux and concentration of each solute. This model was based on the irreversible thermodynamic principles and concentration polarisation theory to only express the water and solute transport through the membrane boundary layer. Therefore, the model ignored the spatial variation of operating parameters along both membrane length and width. The model was validated against experimental

data derived from pretreated palm oil mill effluent as a feed using a hollow fibre membrane module in a pilot plant-scale RO system and showed a high consistency.

Sagne et al. (2009) investigated a one-dimensional (z-axis) dynamic model using the solution-diffusion model to predict the performance of a spiral wound RO process for rejection of five volatile organic compounds (acetic acid, butyric acid, 2-phenylethanol, 2,3-butanediol, and furfural) from dilute aqueous solution from fermentation industries. Unfortunately, the model ignored the impact of the concentration polarisation.

Sundaramoorthy et al. (2011a) and Sundaramoorthy et al. (2011b) suggested a 1D steady state model based on the solution-diffusion model and assumed constant pressure and concentration at the permeate channel. An acceptable convergence was achieved when the model prediction was compared with the experimental data of chlorophenol and dimethylphenol solutes separately.

Fujioka et al. (2014) developed a one-dimensional model (x-axis) based on the irreversible thermodynamic principles of the Spiegler and Kedem model and assumed zero permeate pressure. The model was validated against experimental data of N-nitrosamine rejection from synthesised wastewater.

Al-Obaidi and et al. (2016–2019) developed several robust distributed and lumped models based on solution-diffusion model and irreversible thermodynamic model to estimate the transport phenomena in a spiral wound RO process for the removal of organic pollutants from wastewater. The mathematical models were validated against the experimental work available in the literature.

It is noteworthy to mention that almost all the models developed for predicting the performance of a spiral wound RO process for removing organic chemicals from wastewater have ignored the impact of fouling. This is attributed to a very low feed concentration of these pollutants in industrial wastewater.

The next sections explain in detail the evolution of the spiral wound RO process modelling for wastewater treatment, highlighting model validation against actual experimental data. The next section also presents the models developed for the removal of specific organic and highly toxic compounds from wastewater.

5.6.1 MODEL I: AL-BASTAKI (2004)

Al-Bastaki (2004) developed a lumped model based on the theory of the solution-diffusion model to investigate the efficiency of spiral wound RO membranes for the removal of methyl orange dye and Na_2SO_4 salt from synthetic coloured wastewater under a wide range of operating conditions.

5.6.1.1 Assumptions

- The Debye-Hückel osmotic correlation is used to calculate the osmotic pressure.
- The water permeability constant is expressed in terms of membrane resistance and dynamic membrane resistance.
- Validity of the film theory model to characterise the concentration polarisation.
- The empirical mass transfer expression of a spacer-filled channel developed by Da Costa et al. (1994) is used to calculate the mass transfer coefficient.

5.6.1.2 Model Equations

The solution-diffusion model is applied to express the water and solute transport phenomena. Therefore, the water flux J_w ($\text{kg}_{\text{water}}/\text{m}^2 \text{ s}$) and both methyl orange dye J_d ($\text{kg}_{\text{dye}}/\text{m}^2 \text{ s}$) and Na_2SO_4 salt fluxes J_s ($\text{kg}_{\text{salt}}/\text{m}^2 \text{ s}$), through the membrane are represented as:

$$J_w = A_w (\Delta P_b - \Delta \pi) \quad (5.7)$$

$$J_s = B_s (C_{ws} - C_{ps}) \quad (5.8)$$

$$J_d = B_d (C_{wd} - C_{pd}) \quad (5.9)$$

B_s and B_d are the transport coefficient of salt and dye ($\text{m}^2 \text{ s/kg}$), respectively. The salt and dye concentrations at the membrane wall and permeate side are represented as C_{ws} , C_{wd} , C_{ps} , and C_{pd} (kg/m^3), respectively.

The water permeability constant A_w ($\text{m}^2 \text{ s/kg}$) is estimated based on the resistance of RO membrane R_M ($\text{kg/m}^2 \text{ s}$) and dynamic membrane (formed by the concentrated dye at the membrane wall) R_D ($\text{kg/m}^2 \text{ s}$) (Assumption 3).

$$A_w = \frac{1}{R_M + R_D} \quad (5.10)$$

$$\pi = \frac{\varphi_1 RT_b C_{ws}}{M_s} + \frac{\varphi_2 RT_b C_{wd}}{M_d} \quad (5.11)$$

φ_1 and φ_2 are the Debye-Hückel osmotic coefficients (–) for the salt and dye, respectively (Van Gauwbergen et al., 1997). M_s and M_d are the molecular weight of salt and dye, respectively.

The mass transfer coefficient k (m/s) is estimated using the following correlation of Da Costa et al. (1994)

$$\frac{k d_h}{D_b} = 0.664 k_{dc} \left(\frac{\rho_b d_h U_b}{\mu_b} \right)^{0.5} \left(\frac{\mu_b}{\rho_b D_b} \right)^{0.33} \left(\frac{2d_h}{l_m} \right)^{0.5} \quad (5.12)$$

$$d_h = 2t_f \quad (5.13)$$

d_h , k_{dc} , l_m , and t_f are the hydraulic diameter of the feed spacer channel (m), spacer parameter (–), length of the filament in the spacer mesh (m), and width of feed channel (m), respectively.

Due to the existence of a very low concentration of organic matters in wastewater (dilute aqueous solutions), several researchers have considered the physical property equations of water to be identical for their solutions. Therefore, the correlations of

Koroneos et al. (2007) was used to calculate the physical properties of diffusion coefficient, viscosity, and density. The equations are shown below.

The solute diffusivity of the feed solution and permeate (m^2/s) are given as:

$$D_b = 6.725 \times 10^{-6} \exp \left\{ 0.1546 \times 10^{-3} C_b \times 18.01253 - \frac{2513}{T_b + 273.15} \right\} \quad (5.14)$$

$$D_p = 6.725 \times 10^{-6} \exp \left\{ 0.1546 \times 10^{-3} C_p \times 18.01253 - \frac{2513}{T_p + 273.15} \right\} \quad (5.15)$$

T_b and T_p are the temperature at the feed and permeate channels ($^{\circ}\text{C}$), respectively. The viscosity of feed and permeate ($\text{kg}/\text{m s}$) are:

$$\mu_b = 1.234 \times 10^{-6} \exp \left\{ 0.0212 C_b \times 18.0153 + \frac{1965}{T_b + 273.15} \right\} \quad (5.16)$$

$$\mu_p = 1.234 \times 10^{-6} \exp \left\{ 0.0212 C_p \times 18.0153 + \frac{1965}{T_p + 273.15} \right\} \quad (5.17)$$

The density of feed and permeate (kg/m^3) are:

$$\rho_b = 498.4 m_{f(x)} + \sqrt{248400 m_{f(x)}^2 + 752.4 m_{f(x)} C_{b(x)} \times 18.0153} \quad (5.18)$$

$$\rho_p = 498.4 m_{p(x)} + \sqrt{248400 m_{p(x)}^2 + 752.4 m_{p(x)} C_{p(x)} \times 18.0153} \quad (5.19)$$

$$m_f = 1.0069 - 2.757 \times 10^{-4} T_b \quad (5.20)$$

$$m_p = 1.0069 - 2.757 \times 10^{-4} T_p \quad (5.21)$$

The bulk concentration (kg/m^3) of salt and dye are considered as the average of feed C_f (kg/m^3) and retentate C_c (kg/m^3) concentrations as follows:

$$C_{bs} = \frac{C_{fs} + C_{rs}}{2} \quad (5.22)$$

$$C_{bd} = \frac{C_{fd} + C_{rd}}{2} \quad (5.23)$$

Also, the total and solute material balances give:

$$Q_f = Q_p + Q_r \quad (5.24)$$

$$Q_f C_f = Q_p C_p + Q_r C_r \quad (5.25)$$

Q_f , Q_p , and Q_r are feed, permeate, and retentate flow rates (m^3/s), respectively. C_f , C_p , and C_r are feed, permeate, and retentate concentrations (kg/m^3), respectively. The rejection parameters (–) of salt and dye and the total water recovery are:

$$\text{Rej}_s = \frac{C_{fs} - C_{ps}}{C_{fs}} \quad (5.26)$$

$$\text{Rej}_d = \frac{C_{fd} - C_{pd}}{C_{fd}} \quad (5.27)$$

$$\text{Rec} = \frac{Q_p}{Q_f} \times 100 \quad (5.28)$$

5.6.1.3 Experimentation

Figure 5.2 depicts a schematic diagram of the spiral wound RO process used by Al-Bastaki (2004) to treat coloured wastewater. A polyamide seawater membrane type FilmTec SW30 of an effective membrane area of 2.1 m^2 was applied. The experiments were carried out using different concentrations of methyl orange dye and Na_2SO_4 salt of 0, 500, and 1000 ppm, and 0, 5000, and 10,000 ppm, in aqueous

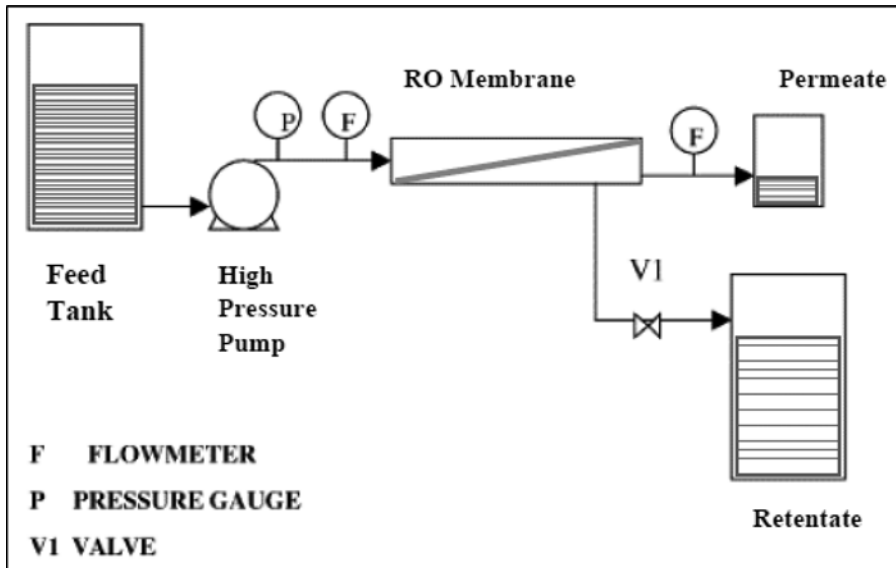


FIGURE 5.2 Schematic diagram of spiral wound RO process.

(Adapted from Al-Bastaki, 2004)

solutions, respectively. Also, the operating pressures of 10, 20, 30, and 40 bar were used to carry out this experiment.

5.6.1.4 Parameters Estimation (Determination of Transport Parameters)

Any mathematical model of an industrial process contains one or several unidentifiable parameters, which cannot be determined from the available observational data. A model-based parameter estimation technique can be used in a systematic and efficient way to estimate those unknown parameters. Murthy and Gupta (1998) used the non-linear parameter estimation method of the Box-Kanemasu to find the model parameters. Senthilmurugan et al. (2005) adopted the simplex search method.

Al-Bastaki (2004) used an iteration method to speculate the salt and dye transport parameters. This is carried out by employing the model together with experimental results. Specifically, an iteration of the salt transport parameter was carried out until the experimental results of solute aqueous solution and theoretical salt rejection and recovery versus pressure curves reached high consistency. The same was repeated to investigate the transport parameter of dye using the experiments of aqueous solution of dye at different pressures. The water transport parameter was obtained from the slope of water flux versus the operating pressure from distilled water (zero osmotic pressure) experiments and based on Eq. (5.1). The membrane resistances were calculated by iteration from experimental results. Table 5.1 shows the values of the unknown model parameters.

5.6.1.5 Model Validation

Figure 5.3 and 5.4 show an acceptable convergence between experimental and model predictions of permeate flux against operating pressure for two sets of experiments. The first experiments used mixtures with 1000 ppm of dye and 5000 ppm and 10,000 ppm of Na₂SO₄. However, the second experiments were carried out for 500 ppm of dye and 5000 ppm and 10,000 ppm of Na₂SO₄. Whilst the model can predict the permeate flux at low operating pressures, it overestimates the permeate flux at high operating pressures.

5.6.2 MODEL II: AHMAD ET AL. (2007)

Ahmad et al. (2007) developed an unsteady state model to estimate the performance of RO membrane to treat a complex multiple organic compounds system. This

TABLE 5.1
Membrane Transport Parameters

Parameter	Unit	Value
A _w	(m ² s/kg)	6.593×10 ⁻¹²
B _s	(m/s)	4.2×10 ⁻⁸
B _d	(m/s)	3.2×10 ⁻⁹
R _M	(kg/m ² s)	1.517×10 ¹¹
R _D	(kg/m ² s)	4.11×1010 e ^{1.25E -7 Pb}

(Adapted from Al-Bastaki, 2004)

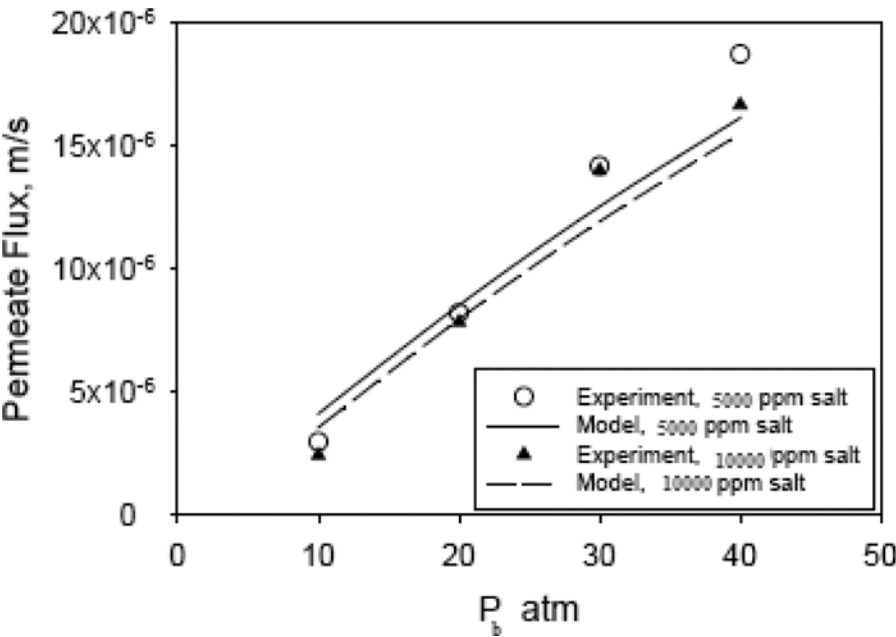


FIGURE 5.3 Model validation against experimental data with 1000 ppm of dye.
(Adapted from Al-Bastaki, 2004)

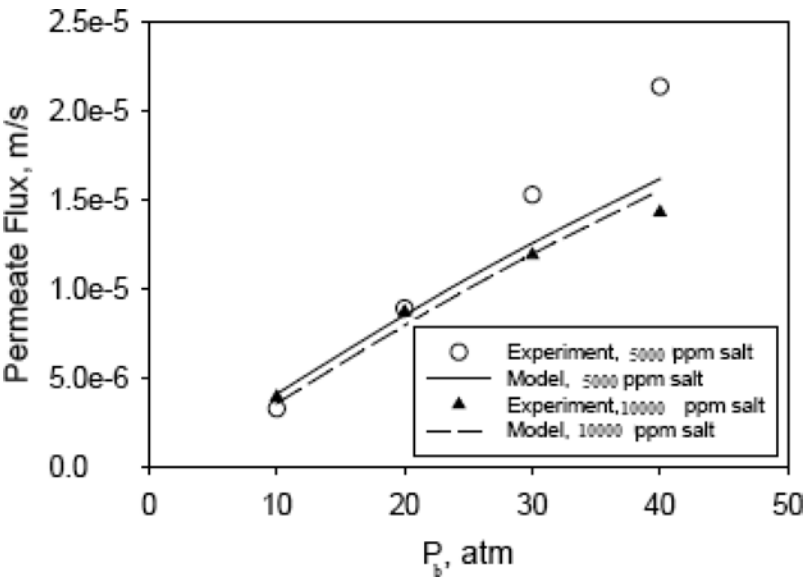


FIGURE 5.4 Model validation against salt experimental data with 500 ppm of dye.
(Adapted from Al-Bastaki, 2004)

resulted in a set of differential equations to express the solutes and water transfer through RO membranes. The model was characterised by coupling the extended Spiegler-Kedem model and concentration polarisation model along the membrane boundary conditions and considering the solute–solute interactions. The model was able to predict the dynamic behaviour of the water flux and rejection of any solute in the multiple solutes system. Moreover, Ahmad et al. (2007) used the chemical oxygen demand (COD) as a guide to study the performance of the RO process.

5.6.2.1 Assumptions

- Validity of Spiegler-Kedem model to express the transport phenomena through RO membrane.
- Validity of the film theory model to characterise the concentration polarisation.
- Fixed operating parameters along the membrane length and width.
- The water and solute fluxes are basically varied along the membrane boundary length (coordinate perpendicular to the membrane, z-axis).
- The solute–solute interactions exist in the multiple solutes system.
- The fluxes of solutes and solvent are extensively linked to the chemical potential differences between the two sides of the membrane.
- Constant membrane transport parameters of water and solutes.
- The underlying process was assumed to be isothermal.

5.6.2.2 Model Equations

The progression of each solute concentration in a multiple solutes system within the concentration polarisation layer of RO membrane can be stated as:

$$\frac{\partial C_i}{\partial t} = -J_w \frac{\partial C_i}{\partial x} + D_b \frac{\partial^2 C_i}{\partial x^2} \quad (5.29)$$

C_i , t , J_w , x , and D_b are solute concentration (kg/m^3), operating time (s), water flux (m/s), the coordinate perpendicular to the membrane (m), and solute diffusivity parameter (m^2/s), respectively.

The water flux in the presence of multiple solutes based on the extended Spiegler-Kedem model of irreversible thermodynamic model, which considers the solute–solute interactions (Ahmad et al., 2005; Al-Obaidi et al., 2017a), can be expressed as:

$$J_w = L_p \left(\Delta P_b - \sum_{i=1}^n \frac{\sigma_i \text{Rej}_i C_{wi} RT_b}{m_i} \right) \quad (5.30)$$

a_i , σ_i , Rej_i , and m_i are the osmotic constant, the reflection coefficient (–) and the intrinsic rejection of the specified solute (–), and the solute molar mass (g/mol), respectively. The intrinsic rejection is defined as:

$$\text{Rej}_i = 1 - \frac{C_{pi}}{C_{wi}} \quad (5.31)$$

However, the observed solute rejection of any solute (–) is given by:

$$Rejo_i = 1 - \frac{C_{pi}}{C_{bi}} \quad (5.32)$$

The observed rejection of any solute can be calculated based on the extended Spiegler-Kedem model for the multiple solutes system where $i = 1, 2, 3, 4, \dots, n$ and $[j = 1, 2, 3, 4, \dots, n \text{ and } j \neq i]$,

$$\frac{1 - R_{eji}}{R_{eji}} = \frac{1 - \sigma_i}{\sigma_i (1 - F_i)} \exp \left(\frac{J_w}{k_i} \right) \quad (5.33)$$

$$F_i = \exp \left[\frac{-J_w (1 - \sigma_i)}{P_{ii}} \left(1 + \sum_{j=1}^n A_j \right) \right] \quad (5.34)$$

$$A_j = \frac{P_{ij} (C_{pj} - C_{bj}) \exp \left(\frac{J_w}{k_j} \right)}{J_w [C_{pi} - (1 - \sigma_i) C_b]} \quad (5.35)$$

$$P_{ii} = \left(\frac{L_{wi}^2}{L_{ww} C_i} - \frac{L_{ii}}{C_i} \right) \frac{RT_b}{\ell m_i} \quad (5.36)$$

$$P_{ij} = \left(\frac{L_{wi} L_{wj}}{L_{ww} C_j} - \frac{L_{ij}}{C_j} \right) \frac{RT_b}{\ell m_j} \quad (5.37)$$

k , P_{ii} , and P_{ij} are the mass transfer coefficient (m/s), the solute permeability coefficient of solute i with the consideration of the interaction of solute i (m/s), and solute permeability coefficient of solute i with the consideration of the interaction of solute j (m/s), respectively. L_{ii} , L_{ww} , L_{wi} , L_{wj} , and L_{ij} are the straight phenomenological coefficient for solute i and solvent (–), cross phenomenological coefficient of solvent–solute i and solute j (–), and cross phenomenological coefficient of solute i and solute j (–), respectively.

The chemical oxygen demand of multiple solutes system is:

$$C_{COD} = \sum_{i=1}^n b_i C_i \quad (5.38)$$

b_i is the dimensionless coefficient.

5.6.2.3 Experimentation

Ahmad et al. (2007) used a pilot plant-scale equipment set-up of the RO process for the treatment of pretreated palm oil mill effluent (POME) discharged from the

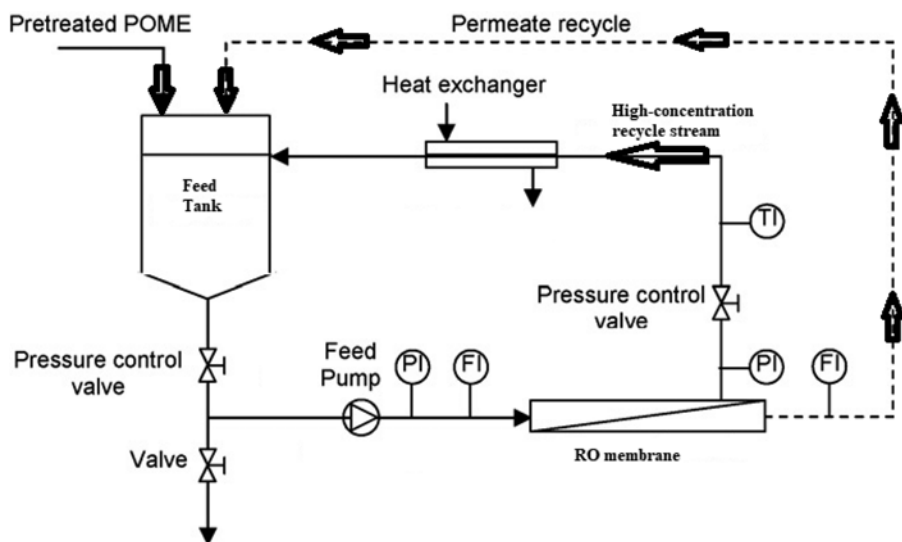


FIGURE 5.5 Schematic diagram of the pilot plant-scale RO process.

(Adapted from Ahmad et al., 2007)

United Palm Oil Mill in Penang, Malaysia. Basically, POME is a very complex mixture of organic matters with an unfriendly odour disposed of from the extraction of palm oil from the fruits as a thick brownish viscous liquid waste of high content of colloidal suspension, BOD, and COD. Specifically, it contains 25,000 mg/L (BOD), 50,000 mg/L COD, 40,500 mg/L (total solids), and 18,000 mg/L (suspended solids), with ammoniacal nitrogen, minerals, carbohydrate constituents, and protein. Figure 5.5 represents the schematic diagram of the RO process used to treat POME. The hollow fibre of RO process type PVDF membrane module B1 (PCI-Memtech) (0.9 m^2 as effective filtration area) was used.

5.6.2.4 Parameters Estimation

The model developed by Ahmad et al. (2007) contains several unknown parameters including σ_i , D_{bi} , P_{ii} , P_{ij} , and viscosity. These parameters were predicted using a non-linear parameter estimation method with Levenberg-Marquardt with Gauss-Newton algorithm (Jain and Gupta, 2004). Table 5.2 presents the results of this optimisation method. However, hydraulic permeability coefficient L_p was allocated via the experiment with deionised water at different operating pressure.

5.6.2.5 Model Validation

Ahmad et al. (2007) compared the simulation results with the actual experimental data of treating POME. This in turn confirmed a satisfactory agreement with the experimental data for the applied pressure between 13.5 to 45.0 bar as depicted in Figure 5.6.

TABLE 5.2
Parameter Estimation Results

Parameter		Value		
L_p (m/Pa s)		9.0096×10^{-12}		
μ (Pa s)		1.024×10^{-3}		
		Solute type		
		[1] Carbohydrate	[2] Ammoniacal nitrogen	[3] Protein
D_{bi} (m ² /s)	3.16×10^{-9}	1.54×10^{-9}	0.67×10^{-9}	
σ_1	0.9998	0.9989	0.9999	
P_{i1} (m/s)	7.345×10^{-9}	4.061×10^{-13}	7.842×10^{-14}	
P_{i2} (m/s)	2.367×10^{-13}	1.484×10^{-12}	1.216×10^{-8}	
P_{i3} (m/s)	3.843×10^{-12}	1.397×10^{-7}	3.633×10^{-12}	

(Adapted from Ahmad et al., 2007)

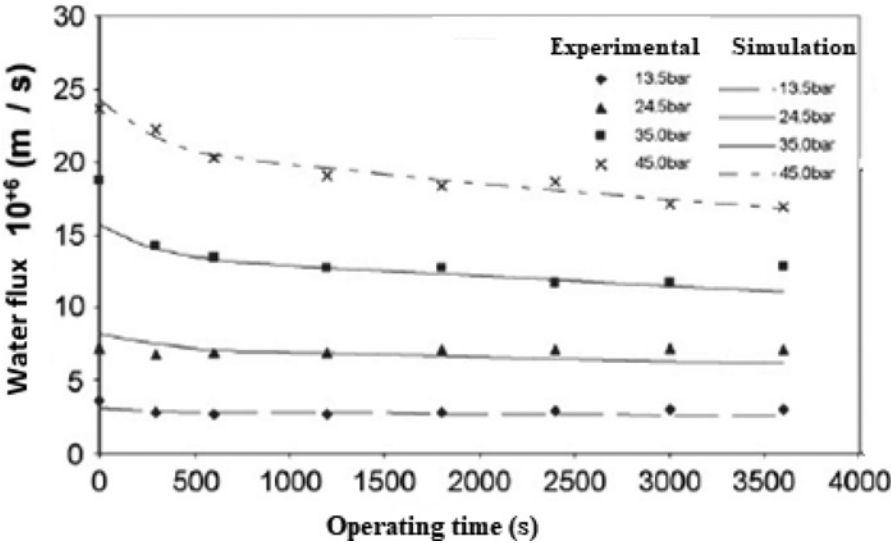


FIGURE 5.6 Model validation of water flux.

(Adapted from Ahmad et al., 2007)

Figure 5.7 presents the comparison of the experimental and simulation results of COD, which shows the successfulness of the model to predict the actual concentration of COD at a high consistency of $R^2 = 0.9911$.

5.6.3 MODEL III: SAGNE ET AL. (2009)

Sagne et al. (2009) developed a dynamic model for estimating the performance of the spiral wound RO process for the removal of a multiple solutes system. For the first time, the model included the solute–solute interaction and identified the variation of retentate and permeate solute concentrations along the z-axis (the coordinate

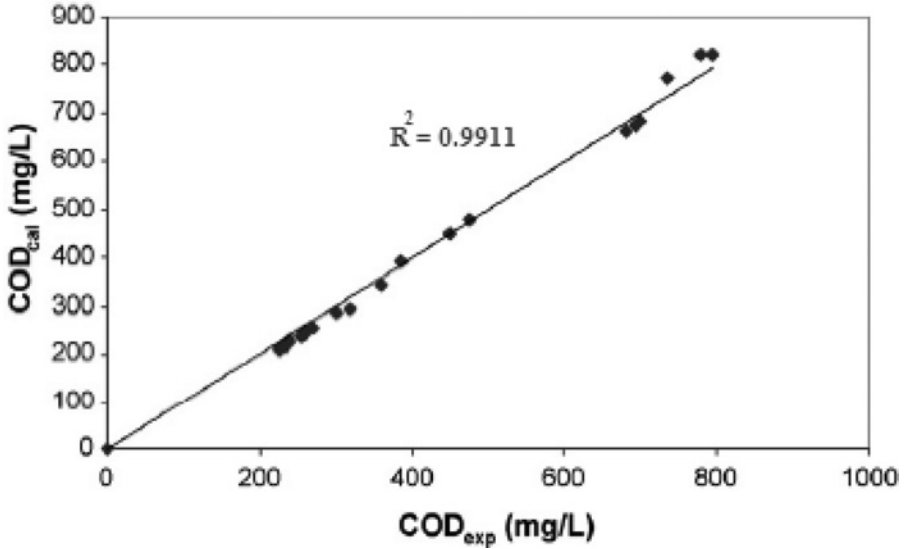


FIGURE 5.7 Experimental vs simulation results of COD.

(Adapted from Ahmad et al., 2007)

perpendicular to the membrane). However, the model ignored the concentration polarisation and the variation of operating parameters along x and y directions in both the feed and permeate channels.

5.6.3.1 Assumptions

- The spiral wound membrane is measured as a flat sheet.
- The spacer size identifies the thickness of both retentate and permeate channels.
- Validity of solution-diffusion model to quantify the transport phenomena through RO membrane.
- The correlation of Langmuir accounts for the relation between the total sorbed quantity of solute and its equilibrium concentration.
- Instantaneous sorption equilibrium is considered between the solution and the membrane.
- No transient phase of the solute and permeate fluxes via the membrane matrix.
- The concentration polarisation is neglected.
- Van't Hoff equation expresses the osmotic pressure.

5.6.3.2 Model Equations

The most important equations are detailed below.

The solute flux (mol/s m²) of any solute in the multiple solutes system is expressed as:

$$J_{si} = \frac{D_{bi} K_{li}}{\delta} (C_{ri} - C_{pi}) \quad (5.39)$$

D_{bi} , K_{li} , and δ are the solute diffusivity (m^2/s), the partition coefficient of solute i between solution and the membrane ($-$), and the membrane thickness (m), respectively. The above equation can be represented as:

$$J_{si} = B_{si} (C_{ri} - C_{pi}) \quad (5.40)$$

Mass balance provides an equation to estimate the total sorbed quantity of solute i (mol/m^2), in equilibrium with equivalent solute concentration at the membrane as:

$$Q_{sori} = \frac{(C_{oi} - C_{eqi})V}{A} \quad (5.41)$$

C_{oi} , C_{eqi} , V , and A are initial solute concentration (mol/m^3), equivalent solute concentration at the membrane (mol/m^3), total treated volume (m^3), and membrane effective area (m^2), respectively. Also, the total sorbed quantity of solute was related to equilibrium solute concentration using the correlation of Langmuir as:

$$Q_{sori} = K_{li} C_{eqi} \quad (5.42)$$

$$Q_{sori} = \frac{Q_{maxi} K_{si} C_{eqi}}{1 + K_{si} C_{eqi}} \quad (5.43)$$

Q_{maxi} and K_{si} are the maximal sorbed quantity of solute (mol/m^2) and the Langmuir equilibrium constant (m^3/mol).

The dynamic variation of retentate and permeate concentrations in the feed and permeate channels are represented as:

$$\frac{\partial C_{ri}}{\partial t} = 1 \frac{1}{t_f \delta} \frac{\partial (C_{ri} F_r)}{\partial y} - \frac{J_{si}}{t_f} = \frac{C_{ri} J_w}{t_f} - \frac{1}{t_f \delta} F_r \frac{\partial C_{pi}}{\partial y} - \frac{j_{si}}{t_f} \quad (5.44)$$

$$\frac{\partial C_{pi}}{\partial t} = 1 \frac{1}{t_p \delta} \frac{\partial (C_{pi} F_p)}{\partial y} - \frac{J_{si}}{t_p} = \frac{C_{pi} J_w}{t_p} - \frac{1}{t_p \delta} F_p \frac{\partial C_{pi}}{\partial y} - \frac{j_{si}}{t_p} \quad (5.45)$$

The retentate and permeate flow rates are linked to permeate flux as:

$$\frac{dF_b}{dy} = -\frac{dF_p}{dy} = -J_w \delta \quad (5.46)$$

Then, a new equation for solute flux was developed based on the membrane thickness, global diffusion constant of solute K_{diffi} (s^{-1}) as:

$$J_{si} = K_{diffi} K_{si} Q_{maxi} \left(\frac{C_{ri}}{1 + K_{si} C_{ri}} - \frac{C_{pi}}{1 + K_{si} C_{pi}} \right) \quad (5.47)$$

$$K_{diffi} = \frac{D_{bi}}{\delta^2} \quad (5.48)$$

Finally, the rejection of any solute is given by:

$$Rej_i = \frac{C_{fi} - C_{pi}}{C_{fi}} \quad (5.49)$$

C_{fi} and C_{pi} are the feed and permeate concentrations (mol/m³), respectively.

5.6.3.3 Experimentation

A brackish water RO aromatic polyamide spiral wound membrane type CPA2 from Hydranautics of 2.6 m² of membrane effective area was used by Sagne et al. (2009) in the treatment of five main solutes particularly found in wastewater. These include acetic and butyric acids, 2,3-butanediol, furfural, and 2 phenylethanol with molecular weight varying between 60.05 and 122.17. These experiments used two types of feed—one synthetic and the other an industrial condensate—to investigate the influence of solute–solute interaction and simulate the original wastewater. A fixed retentate flow rate and an operating temperature of 400 L/h and 20 °C, respectively, were used in the experiments. The process was carried out in a recirculation mode where both retentate and permeate were returned at steady state mode to the feed tank. These were used to investigate the effect of operating pressure (5, 10, 15, 20, and 30 bar) on the process performance. Figure 5.8 shows a schematic diagram of the RO process used.

5.6.3.4 Parameter Estimation

The model developed by Sagne et al. (2009) contains several unknown parameters including K_{diff} , K_{li} , K_{si} , and Q_{max} . These parameters were estimated for each experiment using a multidimensional unconstrained non-linear minimisation method (fminsearch, Matlab, version 7.1), which is constructed in a simplex algorithm

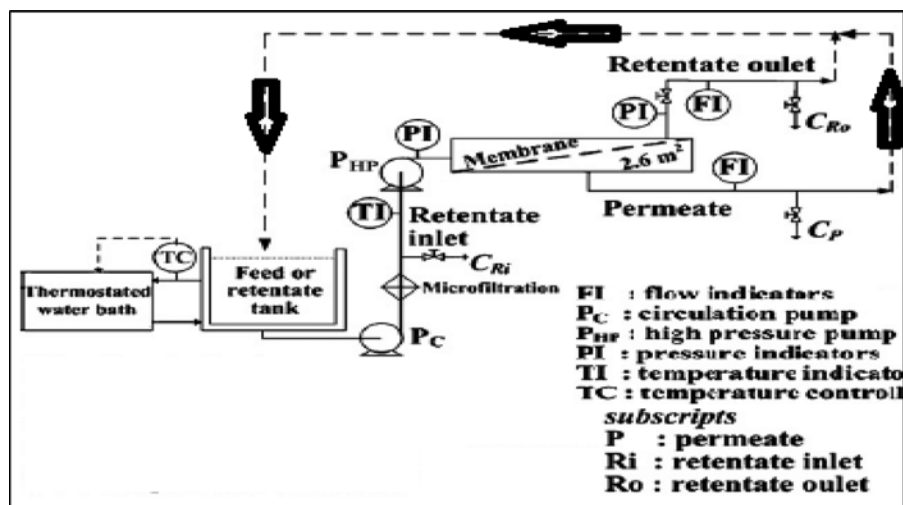


FIGURE 5.8 Schematic diagram of spiral wound RO process.

(Adapted from Sagne et al., 2009)

TABLE 5.3
Estimation of Unknown Parameters

	Solute concentration range (mol/m ³)	Measured $Q_{max,i}$ (mol/m ²)	$K_{s,i}$ (m ³ /mol)	Estimated $K_{diff,i}$ (1/s)	Di (m ² /s)
Acetic acid	0 – 35	–	–	$K_i D = 1.3 \times 10^{-12}$	
Butyric acid	0 – 36	2.5×10^{-2}	1.24×10^{-3}	3.6×10^{-3}	1.44×10^{-16}
Furfural	0 – 0.27	1.1×10^{-3}	4.8	3.41×10^{-3}	1.36×10^{-16}
2,3-Butanediol	0 – 90	–	–	–	–
2-Phenylethanol	0 – 0.18	9.0×10^{-4}	10.5	5.56×10^{-4}	2.22×10^{-17}

(Adapted from Sagne et al., 2009)

(Nelder-Mead). The results of parameter estimation are shown in Table 5.3 for the treatment of a multiple solutes system.

5.6.3.5 Model Validation

Figure 5.9 shows model predictions and the experimental data of the sorption measurements against equivalent concentrations of three selected solutes (butyric acid, furfural, and 2-phenylethanol) performed during batch experiments with the synthetic mixture of these solutes. Figure 5.10 shows the case of only butyric acid in the synthetic condensate wastewater. Interestingly, these figures confirm regression coefficients of over 99%, which clearly evidence the robustness of the model developed.

5.6.4 MODEL IV: SRINIVASAN ET AL. (2009, 2010)

Srinivasan et al. (2009, 2010) developed a simple lumped model based on the solution-diffusion model to characterise the rejection of dimethylphenol and phenol from wastewater using an individual spiral wound RO process.

5.6.4.1 Assumptions

- Constant permeate pressure of 1 atm at the permeate channel.
- Validity of the Van't Hoff relation to express the osmotic pressure.
- Validity of the film theory model to characterise the concentration polarisation.
- Constant values of water and solute transport parameters.
- Constant solute concentrations at the feed and permeate channels.
- The underlying process was assumed to be isothermal.

5.6.4.2 Model Equations

The solvent flux is proportional to the divergence between the hydraulic pressure difference and the osmotic pressure difference across the membrane. However, the

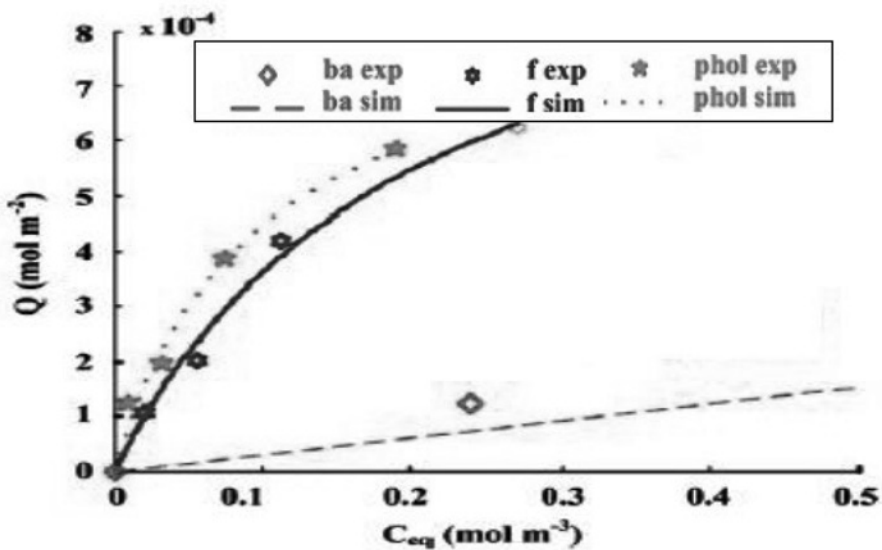


FIGURE 5.9 Sorption isotherms for butyric acid (ba), furfural (f), and 2-phenylethanol (phol) in the synthetic condensate wastewater.

(Adapted from Sagne et al., 2009)

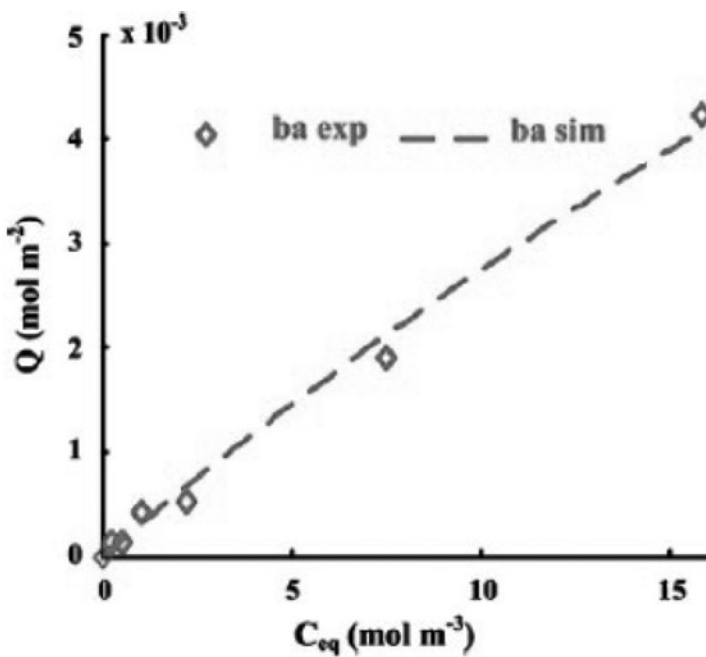


FIGURE 5.10 Sorption isotherm for butyric acid in the synthetic condensate.

(Adapted from Sagne et al., 2009)

solute flux is calculated from the concentration difference across the two sides of the membrane. Therefore, the solvent and solute molar fluxes through the membrane are expressed as follows:

$$J_w = A_w (\Delta P_b - \Delta \pi) \quad (5.50)$$

$$J_s = B_s (C_w - C_p) \quad (5.51)$$

$$\Delta P_b = \left((P_{b(0)} + P_{b(L)}) / 2 - P_p \right) \quad (5.52)$$

$$\Delta \pi = RT_b (C_w - C_p) \quad (5.53)$$

P_p (atm) is the permeate pressure. The accumulated impermeable solute on the membrane surface causes the concentration polarisation layer and can be determined using the stagnant film model proposed by Taniguchi (1978). More specifically, the retained solute accumulates on the membrane wall is greater than the bulk concentration on the high-pressure side of the membrane. Therefore, water flux is linked to the concentration polarisation and mass transfer coefficient k (m/s) (Assumption 3) by the following equation:

$$\frac{(C_w - C_p)}{(C_b - C_p)} = \exp\left(\frac{J_w}{k}\right) \quad (5.54)$$

k is the mass transfer coefficient for the back diffusion of the solute from the membrane to the bulk solution on the high-pressure side of the membrane along the membrane length. The rejection ($-$), bulk, and permeate concentrations are given in the following equations.

$$\text{Rej} = 1 - \frac{C_p}{C_w} \quad (5.55)$$

$$C_b = \frac{C_{b(0)}}{(1 - \tau) + \tau M (1 - \text{Rej})} \quad (5.56)$$

$$\tau = \frac{F_p}{F_{b(0)}} \quad (5.57)$$

$$M = \frac{e^{\frac{J_w}{k}}}{\text{Rej} + (1 - \text{Rej})e^{\frac{J_w}{k}}} \quad (5.58)$$

$$C_p = M C_{b(0)} (1 - \text{Rej}) \quad (5.59)$$

F_b and F_p (m³/s) are the feed flow rate and permeate flow rate, respectively.

5.6.4.3 Experimentation

A pilot-scale crossflow RO filtration system was used by Srinivasan et al. (2009, 2010) in aqueous dimethylphenol and phenol feed solution experiments. The system consisted of a commercial thin-film Perma-TFC polyamide composite RO membrane packed into a spiral wound module (Make: Permionics, Vadodara, India).

Figure 5.11 shows the schematic diagram of the experimental set-up. The characteristics of the spiral wound module are presented in Table 5.4. The experiments of dimethylphenol were carried out for five groups of feed concentrations varying

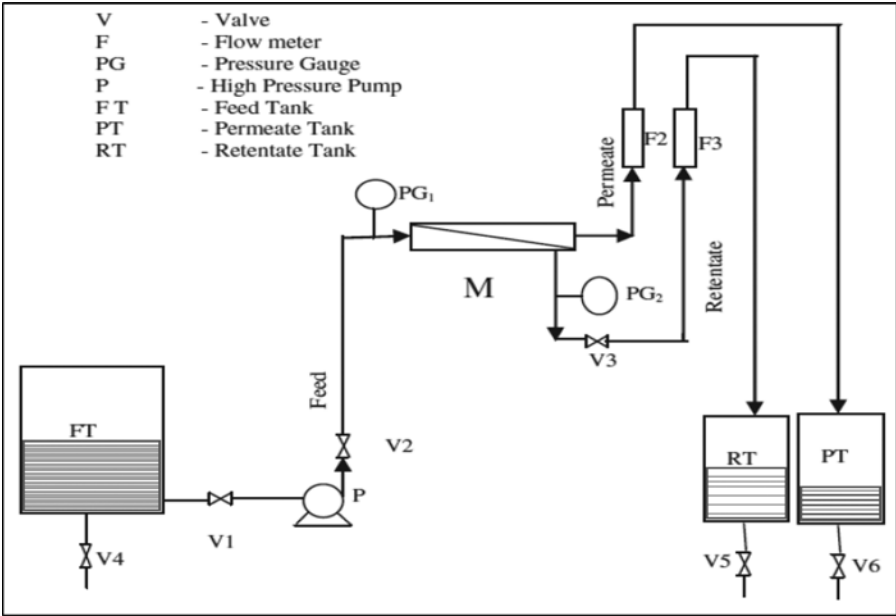


FIGURE 5.11 Schematic diagram of an individual RO process.

(Adapted from Srinivasan et al., 2011)

TABLE 5.4
Membrane Characteristics and Geometry

Property	Value	Property	Value
Manufacturer	Ion Exchange, India	Effective membrane area (A)	0.75 m ²
Membrane material	TFC Polyamide	Module length (L)	0.45 m
Module configuration	Spiral wound	Module width (W)	1.67 m
Feed spacer thickness (<i>t_f</i>)	0.85 mm	Module diameter	64.52 mm
Permeate channel thickness (<i>t_p</i>)	0.78 mm		

(Adapted from Srinivasan et al., 2011)

between 2.125E-3 and 10.6E-3 kmol/m³. For each group of inlet feed concentration, the experiments were carried out for a set of feed pressure varied between 4.93 to 14.8 atm and temperature between 31.5 to 34.5 °C. Phenol experiments were carried out for five groups of feed concentrations varying between 0.69E-3 and 6.33E-3 kmol/m³. They were carried out for a set of feed pressure varying between 4.9 and 11.76 atm and a temperature varying between 32 and 38 °C for each group of feed concentration. The feed was pumped in a constant feed flow rate of 3.33E-4 m³/s in both the dimethylphenol and phenol experiments.

5.6.4.4 Parameter Estimation

Srinivasan et al. (2009, 2010) used the graphical method developed by Murthy and Gupta (1999) for the determination of the unknown parameters for their proposed model. The estimated model transport parameters (A_w and B_s) are given in Table 5.5.

5.6.4.5 Model Validation

The model developed by Srinivasan et al. (2009, 2010) has been validated against the experimental data of dimethylphenol (Srinivasan et al., 2009) and phenol (Srinivasan et al., 2010) removal from wastewater. A maximum error of 18.8% was found in estimating the permeate concentration of dimethylphenol with low errors for the estimation of the rejection rate. However, the model shows a maximum error of 13.5% for predicting the rejection of phenol compared to experimental data.

5.6.5 MODEL V: SUNDARAMOORTHY ET AL. (2011A)

A one-dimensional steady state model (1D) has been developed for an individual spiral wound RO process by Sundaramoorthy et al. (2011a) based on the solution-diffusion model. The model was able to predict the spatial variation of operating parameters along the membrane length. This is compared to the model developed by Srinivasan et al. (2009, 2010), which is built on lumped conditions where the spatial variation of concentration and pressure on feed and permeate channels were not taken into consideration.

TABLE 5.5
Results of Parameter Estimation

Solute	Parameter	Value
Dimethylphenol	A_w	8.6428E-7 (m/atm s)
	B_s	1.1822E-7 (m/s)
Phenol	A_w	5.9393E-7 (m/atm s)
	B_s	6.5367E-7 (m/s)

(Adapted from Srinivasan et al., 2009, 2010)

5.6.5.1 Assumptions

The assumptions of the model of Srinivasan et al. (2009, 2010) were valid except for the relaxation of the constant feed concentration at the feed channel. The following assumptions were made to develop the model:

- A flat membrane sheet with negligible channel curvature.
- Validity of Darcy's law for the feed channel where the friction parameter is applied to characterise the pressure drop.
- Validity of the film model theory to estimate the concentration polarisation impact.
- Constant permeate concentration at the permeate channel.
- Constant 1 atm pressure at the permeate side.
- Solvent and solute transport parameters and friction factor are constant.
- Isothermal process and where the temperatures of the feed, brine, and permeate are equal.

5.6.5.2 Model Equations

The water flux and feed pressure at any point along the x-axis are represented as:

$$J_{w(x)} = \frac{\emptyset}{A \sinh \emptyset} \left[\left(F_{b(0)} \cosh \emptyset \left(1 - \frac{x}{L} \right) - F_{b(L)} \cosh \frac{\emptyset x}{L} \right) \right] \quad (5.60)$$

$$\emptyset = L \left(\frac{WbA_w}{\left(1 + A_w \frac{R}{B_s} TC_p \right)} \right)^{0.5} \quad (5.61)$$

$$P_{b(x)} = P_{b(0)} - \frac{bL}{\emptyset \sinh \emptyset} \left[F_{b(L)} \left(\cosh \frac{\emptyset x}{L} - 1 \right) - F_{b(0)} \left(\cosh \emptyset \left(1 - \frac{x}{L} \right) - \cosh \emptyset \right) \right] \quad (5.62)$$

b is the feed channel friction parameter (atm s/m⁴). The retentate pressure (at $x = L$) is:

$$P_{b(L)} = P_{b(0)} - \frac{bL}{\emptyset \sinh \emptyset} \left[\left(F_{b(0)} + F_{b(L)} \right) (\cosh \emptyset - 1) \right] \quad (5.63)$$

The osmotic pressure at any point along the x-axis is:

$$\Delta \pi_{(x)} = R(T_b + 273.15) (C_{b(x)} - C_p) \quad (5.64)$$

The bulk concentration at any point along the x-axis is:

$$C_{b(x)} = C_p + \frac{F_{b(0)} (C_{b(0)} - C_p)}{F_{b(x)}} \quad (5.65)$$

The rejection parameter is:

$$Rej = 1 - \frac{C_p}{C_{b(L)}} \quad (5.66)$$

The mass transfer coefficient of dimethylphenol and chlorophenol at any point along the x-axis are given by Eqs. (5.67) and (5.68), respectively:

$$k_{(x)} de_b = 246.9 D_{b(x)} Re_{b(x)}^{0.101} Re_{p(x)}^{0.803} C_{m(x)}^{0.129} \quad (5.67)$$

$$k_{(x)} de_b = 147.4 D_{b(x)} Re_{b(x)}^{0.13} Re_{p(x)}^{0.739} C_{m(x)}^{0.135} \quad (5.68)$$

Reynolds number (–) on the feed and permeate channels are calculated from the following equations:

$$Re_{b(x)} = \frac{\rho_{b(x)} de_b F_{b(x)}}{t_f W \mu_{b(x)}} \quad (5.69)$$

$$Re_{p(x)} = \frac{\rho_{p(x)} de_p J_{w(x)}}{\mu_{p(x)}} \quad (5.70)$$

de_b and de_p (m) are the equivalent diameters of the feed and permeate channels, respectively. $C_{m(x)}$ is the dimensionless solute concentration at any point along x-axis.

$$de_b = 2t_f \quad (5.71)$$

$$de_p = 2t_p \quad (5.72)$$

$$C_{m(x,y)} = \frac{C_{b(x,y)}}{\rho_w} \quad (5.73)$$

t_f and t_p (m) are the height of feed channel and permeate channel, respectively. ρ_w is the molal density of water.

Finally, the permeate concentration at any point along the permeate channel is:

$$C_p = \frac{C_{b(x)}}{\left(\frac{J_{w(x)}}{1 + \frac{B_s}{e^{\frac{J_{w(x)}}{k_f(x)}}}} \right)}$$

(5.74)

5.6.5.3 Experimentation

Sundaramoorthy et al. (2011b) and Srinivasan et al. (2011) used the same laboratory pilot-scale crossflow RO filtration system shown in Figure 5.11 in their experimental work to remove chlorophenol and dimethylphenol from aqueous solutions of different concentrations. They also used the same commercial thin-film composite RO membrane packed into a spiral wound module (Ion Exchange, India Ltd.), but with an effective membrane area of 7.85 m² as reported in the characteristics of the module used and shown in Table 5.6. The solute concentrations varied from 0.778E-3 to 6.548E-3 kmol/m³. The feed was pumped at three flow rates of 2.166E-4, 2.33E-4, and 2.583E-4 m³/s with feed pressures varying from 5.83 to 13.58 atm for each selected feed flow rate.

5.6.5.4 Parameter Estimation

Sundaramoorthy et al. (2011a) developed a new graphical method for predicting the model unknown parameters, including water *A_w* and solute *B_s* transport parameters and the friction factor *b*. Table 5.7 shows the parameters considering the membrane

TABLE 5.6
Membrane Characteristics and Geometry

Property	Value	Property	Value
Maker and configuration	Ion Exchange, India Ltd., TFC Polyamide, spiral wound	Module diameter	0.0825 (m)
Feed (t _f) and permeate (t _p) channel thickness	0.8 (mm) and 0.5 (mm)	Maximum operating temperature (°C)	40
Module length (L) and width (W)	0.934 (m) and 8.4 (m)	Maximum operating pressure (atm, bar)	24.772, 25.1
Membrane volume	6.276E-3 m ³	Maximum pressure drop per element (atm, bar)	1.382, 1.4
Effective membrane area (A)	7.85 m ²	Maximum and minimum feed flow rate (m ³ /s)	1E-4–1E-3

(Adapted from Srinivasan et al., 2011)

TABLE 5.7
Results of Parameter Estimation Measured at 30–32 °C

Solute	Parameter	Value
Chlorophenol	b	$8529.45 \left(\frac{\text{atm s}}{\text{m}^4} \right)$
	A_w	$9.5188\text{E-}7 \left(\frac{\text{m}}{\text{atm s}} \right)$
	B_s	$8.468\text{E-}8 \left(\frac{\text{m}}{\text{s}} \right)$
Dimethylphenol	b	$9400.9 \left(\frac{\text{atm s}}{\text{m}^4} \right)$
	A_w	$9.7388\text{E-}7 \left(\frac{\text{m}}{\text{atm s}} \right)$
	B_s	$1.5876\text{E-}8 \left(\frac{\text{m}}{\text{s}} \right)$

(Adapted from Sundaramoorthy et al. (2011a)

type Ion Exchange, India for the experiments of chlorophenol and dimethylphenol removal from wastewater.

5.6.5.5 Model Validation

The model developed was validated against the experimental data of Sundaramoorthy et al. (2011b) for chlorophenol and Srinivasan et al. (2011) for dimethylphenol removal from wastewater. An accepted convergence was achieved when the model prediction was compared with experimental data of chlorophenol and dimethylphenol solutes separately. Maximum errors of 15.4% and 13.8% were found in estimating the permeate concentration of chlorophenol and dimethylphenol respectively with a large range of low errors associated with the other operating parameters of retentate feed flow rate and rejection parameter. The assumption of constant transport parameters in the model of Sundaramoorthy et al. (2011a) has reduced the accuracy of model prediction against experimental data. However, it can be said that the model was able to estimate the performance of an individual spiral wound module of RO process with sufficient accuracy compared to that of the lumped parameter model (Srinivasan et al., 2009).

5.6.6 MODEL VI: FUJIOKA ET AL. (2014)

A comprehensive work to investigate the performance of a full-scale multi-stage spiral wound RO plant was carried out by Fujioka et al. (2014), who developed a specific one-dimensional (1D) model based on the irreversible thermodynamics principle and

the hydrodynamic calculations to investigate the total N-nitrosamine rejection from wastewater.

5.6.6.1 Assumptions

- The pressure drop in the feed section was identified using the Schock and Miquel model.
- Local permeate pressure at the permeate channel was assumed equal to zero.
- The underlying process was assumed to be isothermal.

5.6.6.2 Model Equations

The water flux at any point along the x-axis is calculated as:

$$J_{w(x)} = L_p \left[\left(P_{b(x)} - P_p - \sigma \Delta \pi_{(x)} \right) \right] \quad (5.75)$$

The permeate flux per each slide and total permeate flux (m³/s) of membrane are:

$$Q_{p(x)} = J_{w(x)} \Delta S \quad (5.76)$$

$$Q_{p,t} = \sum Q_{p(x)} \quad (5.77)$$

The osmotic pressure at each point along the x-axis is:

$$\pi_{(x)} = 1.19 (T + 273.15) \sum C_{b(x)} \quad (5.78)$$

The bulk concentration is usually increased along the feed channel. Eq. (5.79) is used to calculate the progress of feed concentration at any point along the x-axis:

$$C_{b(x+1)} = \frac{F_{b(x)} C_{b(x)} - C_{p(x)} Q_{p(x)}}{F_{b(x+1)}} \quad (5.79)$$

The material balance of any selected sub-section along the feed channel feed flow rate gives Eq. (5.80). This can be used to estimate the feed flow rate at any point along the x-axis as:

$$F_{b(x+1)} = F_{b(x)} - Q_{p(x)} \quad (5.80)$$

The pressure drop at any point along the membrane length and the total pressure drop per each element are calculated as:

$$\Delta P_{b(x)} = 0.5 b \rho_{b(x)} U_{b(x)}^2 \frac{\Delta x}{d_h} \quad (5.81)$$

$$\Delta P_{b,t} = \sum \Delta P_{b(x)} \quad (5.82)$$

$U_{b(x)}$ is the bulk feed velocity at any point along x-axis of the feed channel (m/s). In this respect, the progress of feed pressure at any selected sub-section along the membrane length is evaluated as:

$$P_{b(x+1)} = P_{b(x)} - \Delta P_{b(x)} \quad (5.83)$$

The physical property of fluid viscosity is:

$$\mu_b = 2.141E - 5 \times 10^{\left(\frac{247.8}{(T_b + 273.15) - 140}\right)} \quad (5.84)$$

The rejection and observed rejection Rej_{obs} (–) parameters at any point along the membrane length is:

$$Rej_{(x)} = \frac{\sigma(1 - F_{(x)})}{(1 - \sigma F_{(x)})} \quad (5.85)$$

$$Rej_{obs(x)} = \frac{Rej_{(x)}}{(1 - Rej_{(x)}) \times \exp\left(\frac{J_{w(x)}}{k_{(x)}}\right) + Rej_{(x)}} \quad (5.86)$$

The parameter ($F_{(x)}$) is calculated by Eq. (5.87) as follows:

$$F_{(x)} = \exp\left[-\frac{(1 - \sigma)}{B_s} J_{w(x)}\right] \quad (5.87)$$

The mass transfer coefficient of N-nitrosamine at any point along the membrane length is related to physical properties and the efficiency of mixing ($K = 0.5$) and is expressed as:

$$k_{(x)} = 0.753 \left(\frac{K}{2 - K}\right)^{0.5} \left(\frac{D_{b(x)}}{t_f}\right) \left(\frac{\mu_{b(x)} \rho_{b(x)}}{D_{b(x)}}\right)^{0.1666} \left(\frac{2 t_f^2 U_{b(x)}}{D_{b(x)} \Delta L}\right)^{0.5} \quad (5.88)$$

Eqs. (5.89) and (5.90) are used to calculate the permeate concentration and the overall permeate concentration at any point along the permeate channel as follows:

$$C_{p(x)} = C_{b(x)} (1 - Rej_{obs}) \quad (5.89)$$

$$C_{p(av)} = \frac{\sum C_{p(x)} Q_{p(x)}}{\sum Q_{p(x)}} \quad (5.90)$$

5.6.6.3 Experimentation

A full-scale RO filtration system of three and seven 4-inch glass-fibre pressure vessels shown in Figure 5.12 and 5.13, respectively, were used by Fujioka (2014) in the

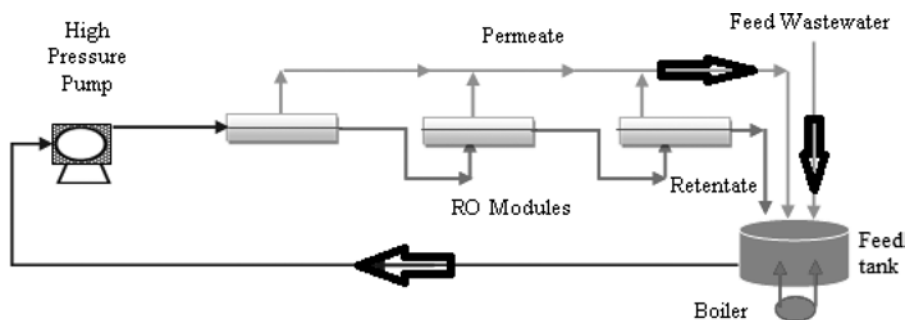


FIGURE 5.12 Schematic diagram of full-scale three-element RO plant.

(Adapted from Al-Obaidi et al., 2018c)

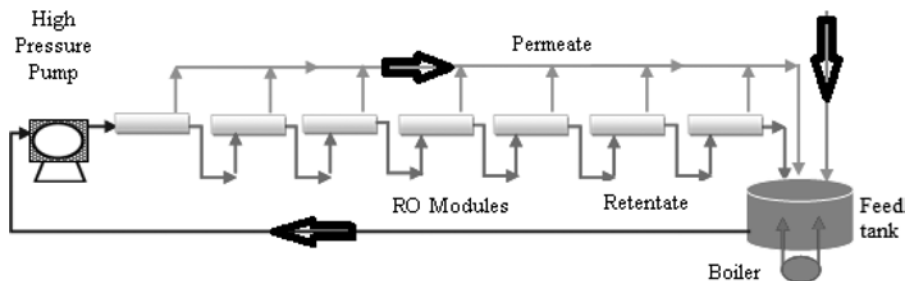


FIGURE 5.13 Schematic diagram of full-scale seven-element RO plant.

(Adapted from Al-Obaidi et al., 2017g)

experiments of eight N-nitrosamine solutes rejection with a molecular weight in the range of 74 to 158 g/mol.

The N-nitrosamine stock solutions were prepared in pure methanol and contained 10 mg/L of each N-nitrosamine solute in the tested solution (pH 8.0) (N-nitrosodimethylamine-D6 [NDMA], N-nitrosomethylethylamine-D3 [NMEA], N-nitrosopyrrolidine-D8 [NPYR], N-nitrosodiethylamine-D10 [NDEA], N-nitrosopiperidine-D10 [NPIP], N-nitrosomorpholine-D8 [NMOR], N-nitrosodipropylamine-D14 [NDPA], and N-nitrosodi-n-butylamine-D9 [NDBA]) as summarised in Table 5.8.

Also, an aqueous feed of stock solutions of NaCl, CaCl₂, and NaHCO₃ were prepared in Milli-Q water at 2M (NaCl) and 0.1 M (CaCl₂ and NaHCO₃) to simulate the electrolyte composition typically found in treating wastewater. The filtration experiments were carried out by introducing the stock solution of N-nitrosamine in the feed to obtain approximately 250 ng/L of each target N-nitrosamine.

The feed was pumped using a high-pressure pump type (Hydra-Cell, Wanner Engineering Inc., Minneapolis, MN, USA) at constant volumetric feed flow rate of 2.43E-3 m³/s, while the average permeate flux was adjusted at 2.78E-6, 5.56E-6, and 8.33E-6 m/s during the experiments by increasing the operating feed pressure from

TABLE 5.8**Physical and Transport Parameters of the Eight N-nitrosamines**

Name	Molecular weight (g/mol)	Inlet feed concentration, $C_{b(0)}$ $\times E+9$ (kmol/m ³)	Solute permeability coefficient, B_s (m/s) at 20 °C	Reflection coefficient, σ (–)
NDBA	158.1	1.581	4.33E-8	0.990
NDEA	102.1	2.449	2.26E-7	0.985
NDMA	74.1	3.376	5.35E-6	0.953
NDPA	130.1	1.921	6.02E-8	0.992
NMEA	88.1	2.839	1.14E-6	0.958
NMOR	116.1	2.154	2.06E-7	0.991
NPIP	114.1	2.191	9.25E-8	0.993
NPYR	100.1	2.499	5.12E-7	0.973

Pure water permeability at 20 °C $L_p = 5.2$ (∓ 0.2) L/m² h bar

(Adapted from Al-Obaidi et al., 2018c)

TABLE 5.9**Specifications of the Spiral Wound Membrane Element**

Property	Value
Manufacturer	Hydranautics, Oceanside, CA, USA
Membrane type and configuration	ESPA2–4040, Spiral Wound, Composite Polyamide
Feed and permeate spacer thickness t_f and t_p (m)	6.6E-4
Membrane sheet area (m ²)	7.9
Membrane sheet length L (m)	0.9
Membrane sheet width W (m)	8.778
Characteristic length of spacer ΔL (m)	0.006
The efficiency of mixing K (dimensionless) *	0.5
Diffusion coefficient of NDMA D_b at 20 °C (m ² /s)	9.7E-10
Maximum applied pressure (atm, bar)	41.1, 41.6
Maximum operating temperature (°C)	45

* Mane et al. (2009)

(Adapted from Al-Obaidi et al., 2018c)

4, 6.5, and 10.1 atm. The feed solution temperature was kept along the experiments at 20 ± 0.1 °C using a chiller/heater unit type (Neslab RTE 7, Thermo Scientific Inc., Waltham, MA, USA). Each pressure vessel holds only one spiral wound element type ESPA2–4040 (Make: Hydranautics, Oceanside, CA, USA).

The pressure vessels were connected in series, where the concentrated feed solution of the first vessel was transferred to the second vessel followed by the third one. The feed tank (0.3 m³) in Figures 5.12 and 5.13 was filled in with the model

wastewater at the beginning of the process. After the process was started, the collected permeate and retentate were circulated back to the feed reservoir to maintain constant feed concentration. The experimental work of Fujioka (2014) considered a very low concentration of N-nitrosamine. Therefore, the physical properties of diffusivity, density, and viscosity have been assumed identical to water equations. The specifications of the spiral wound membrane element are given in Table 5.9.

5.6.6.4 Parameter Estimation

Fujioka (2014) used an iteration procedure to minimise the difference between the model prediction and the observed feed pressure to characterise the unknown friction parameter of the model. This method yielded the values of feed friction parameters of 3.9, 4.3, and 5.5 at permeate flow rate of 2.78E-6, 5.56E-6, and 8.33E-6 m/s, respectively. However, the water and solute permeability constants and the reflection coefficient of each solute were calculated experimentally and are given in Table 5.8.

5.6.6.5 Model Validation

Figures 5.14 and 5.15 show the comparison between the model predictions and the experimental data of the pressure variation along the membrane length (series of three membranes) and the rejection of three tested N-nitrosamine compounds, respectively. The model prediction was almost consistent with the experimental results, especially at low and medium feed pressures. However, the model overestimated the rejections, especially those of NDMA. This was probably caused by inaccurately estimating its solute transport parameter value.

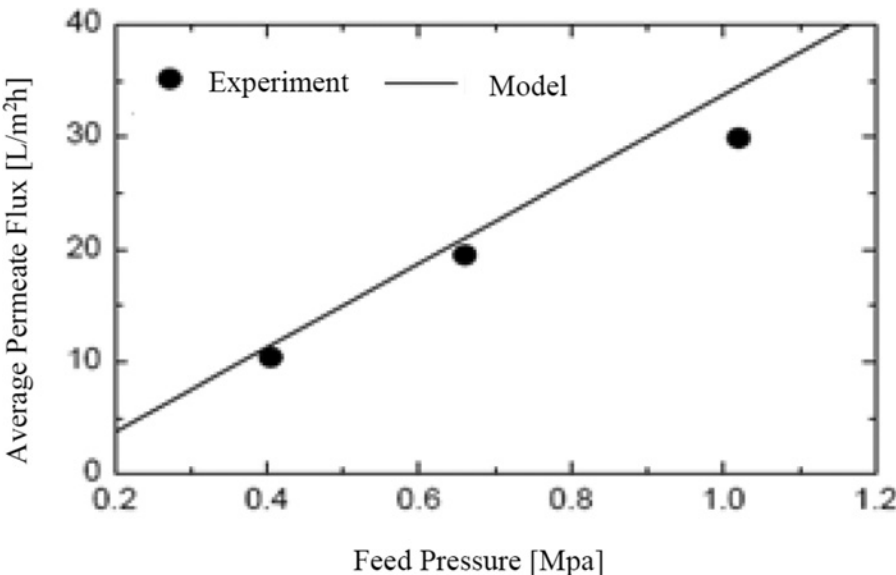


FIGURE 5.14 Permeate flux vs feed pressure.

(Adapted from Fujioka et al., 2014)

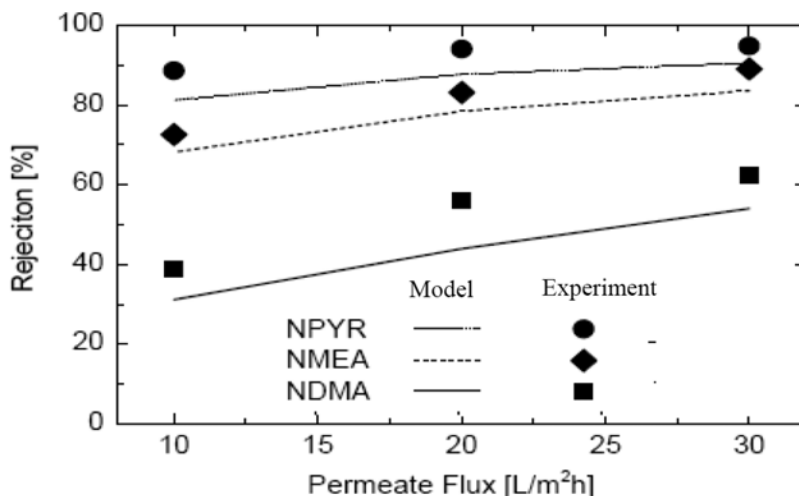


FIGURE 5.15 Model prediction and observed permeate flux of three membranes.

(Adapted from Fujioka et al., 2014)

The results indicate the importance of having an accurate model together with a reliable process design, which can be used to describe the process more accurately. Al-Obaidi et al. (2016) developed several methods (as described later) which resolve, to a large extent, the critical issue of providing spatial modelling under steady state and dynamic conditions.

5.6.7 MODEL VII: AL-OBALDI AND MUJTABA (2016)

A mathematical one-dimensional steady and dynamic model applicable for dilute binary aqueous solution in a spiral wound RO process has been developed by Al-Obaidi and Mujtaba (2016). The model relaxed the assumptions of constant physical properties and concentration of the fresh water on the permeate side. Moreover, the retentate concentration varied along the membrane length (one-dimensional model) due to the impact of both plug flow and diffusion flow. A number of explicit differential equations were developed to predict the flow rate, concentration, pressure, and temperature at each point along the feed and permeate channels length in respect of the operating time. This model could readily predict the dynamic behaviour of water flux, solute flux, and solute concentration on the wall of the membrane. Also, the model takes into consideration the impact of concentration, pressure, and temperature on the physical properties of the solution yielding a variable mass transfer coefficient and concentration polarisation. This is due to the prediction made on the variation of the operating parameters along the membrane length. This model can in fact deal with any organic compound with the appropriate mass transfer coefficient model.

5.6.7.1 Assumptions

The assumptions made by Sundaramoorthy et al. (2011a) are also used in this model, with the exception of the constant permeate concentration at the permeate channel, which was relaxed. Therefore, the following assumptions were considered to build the model:

- The principles of the solution-diffusion model were used to express the mass transport through the membrane.
- A flat membrane sheet with fixed membrane characteristics and negligible channel curvature.
- Validity of Darcy's law for the feed channel where the friction parameter is applied to characterise the pressure drop.
- Validity of the film model theory to estimate the concentration polarisation impact.
- Constant atmospheric pressure at the permeate side.
- The permeate concentration is varied along the membrane length, but the mean value is considered as the freshwater output concentration for the calculation of the whole unit solute rejection. This is attributed to the direction of the accumulated permeate flow rate, which is in the spiral direction.
- Solvent and solute transport parameters and friction factor are constant.
- The bulk concentration varies only along the membrane length (x-axis) due to the impact of both plug flow and diffusion flow.
- The physical properties vary along the feed and permeate channels.
- Negligible impact of feed spacer on the fluid patterns at the feed channel.
- Constant friction factor of feed channel is assumed due to the laminar flow.

Note, the spiral wound membrane is basically treated as unwound, which has a similar configuration of the plate and frame module. This assumption, which is used to simplify the complex configuration of a spiral wound RO module, has also been used by several researchers including Senthilmurugan et al. (2005) and Sundaramoorthy et al. (2011a). In this respect, Gu et al. (2017) developed a successful one-dimensional model despite neglecting the presence of the feed spacer. This model was validated against the experimental data of seawater desalination as opposed to wastewater treatment.

5.6.7.2 Model Equations

The water and solute fluxes are given by:

$$J_{w(x)} = A_w \left((P_{b(x)} - P_p) - RT_{b(x)} (C_{w(x)} - C_{p(x)}) \right) \quad (5.91)$$

$$J_{s(x)} = B_s \exp \left(\frac{J_{w(x)}}{k_{(x)}} \right) (C_{b(x)} - C_{p(x)}) \quad (5.92)$$

The solute concentration at any point along the membrane surface is calculated based on the film theory as:

$$\frac{(C_{w(x)} - C_{p(x)})}{(C_{b(x)} - C_{p(x)})} = \exp\left(\frac{J_{w(x)}}{k_{(x)}}\right) \quad (5.93)$$

The total (whole module) mass and solute balance can be presented as:

$$F_{b(0)} = F_{b(x)} + F_{p(x)} \quad (5.94)$$

$$F_{b(0)} C_{b(0)} = F_{b(x)} C_{b(x)} + F_{p(x)} C_{p(x)} \quad (5.95)$$

The variation of retentate flow rate along x-axis can be estimated with the water flux through the membrane using:

$$\frac{dF_{b(x)}}{dx} = -\frac{dF_{p(x)}}{dx} = -W J_{w(x)} \quad (5.96)$$

W (m) is the width of membrane. Also, the permeate flow rate for each sub-section is:

$$F_{p(x)} = J_{w(x)} W \Delta x \quad (5.97)$$

Δx (m) is the length of the sub-section. The pressure drop along the length of the membrane can be accounted from the momentum balance equation, which is based on Darcy's law (second assumption) where the pressure loss is caused by the wall friction along the membrane.

$$\frac{dP_{b(x)}}{dx} = -b F_{b(x)} \quad (5.98)$$

5.6.7.2.1 The Conservation Equations of the Dynamic Model

The retentate concentration varies along the membrane length due to the impact of the plug flow and diffusion terms. The variations of retentate and permeate concentrations along the feed channel length and permeate channel length against operating time (1D dynamic model) are estimated by:

$$\frac{dC_{b(x)}}{dt} = -\frac{C_{b(x)}}{t_f W} \frac{dF_{b(x)}}{dx} - \frac{F_{b(x)}}{t_f W} \frac{dC_{b(x)}}{dx} + \frac{d}{dx} \left[D_{b(x)} \frac{dC_{b(x)}}{dx} \right] - \frac{J_{w(x)} C_{p(x)}}{t_f} \quad (5.99)$$

$$\frac{dC_{p(x)}}{dt} = -\frac{C_{p(x)}}{t_p W} \frac{dF_{p(x)}}{dx} - \frac{F_{p(x)}}{t_p W} \frac{dC_{p(x)}}{dx} + \frac{d}{dx} \left[D_{p(x)} \frac{dC_{p(x)}}{dx} \right] + \frac{J_{w(x)} C_{p(x)}}{t_f} \quad (5.100)$$

As can be seen from Eqs. (5.99) and (5.100), the dynamic behaviour of both feed and permeate concentrations is controlled by the flux of solute penetrate the membrane. Also, the dynamic behaviour of retentate flow rate, retentate pressure are estimated from:

$$\frac{dF_{b(x)}}{dt} = \left[\left\{ -W \left(A_w \left((P_{b(x)} - P_p) - RT_{b(x)} \exp \left(\frac{J_{w(x)}}{k_{(x)}} \right) (C_{b(x)} - C_{p(x)}) \right) \right) \right\} - \frac{dF_{b(x)}}{dx} \right] \left(\frac{F_{b(x)}}{t_f W} \right) \quad (5.101)$$

$$\frac{dP_{b(x)}}{dt} = \left[\left\{ (-bF_{b(x)}) \right\} - \frac{dP_{b(x)}}{dx} \right] \left(\frac{F_{b(x)}}{t_f W} \right) \quad (5.102)$$

The water and solute fluxes through the membrane and wall concentration are:

$$\frac{dJ_{w(x)}}{dt} = \left\{ \left(A_w \left((P_{b(x)} - P_p) - RT_{b(x)} (C_{w(x)} - C_{p(x)}) \right) \right) - J_{w(x)} \right\} \left(\frac{F_{b(x)}}{t_f W \Delta x} \right) \quad (5.103)$$

$$\frac{dJ_{s(x)}}{dt} = \left\{ \left(B_s \exp \left(\frac{J_{w(x)}}{k_{(x)}} \right) (C_{b(x)} - C_{p(x)}) \right) - J_{s(x)} \right\} \left(\frac{F_{b(x)}}{t_f W \Delta x} \right) \quad (5.104)$$

$$\frac{dC_{w(x)}}{dt} = \left\{ \left(C_{p(x)} + \exp \left(\frac{J_{w(x)}}{k_{(x)}} \right) (C_{b(x)} - C_{p(x)}) \right) - C_{w(x)} \right\} \left(\frac{F_{b(x)}}{t_f W \Delta x} \right) \quad (5.105)$$

The last set of equations contains the energy balance dynamic equations of retentate and permeate temperatures along the length of the membrane. By assuming a well-insulated system, the following equations can be drawn:

$$\frac{dT_{b(x)}}{dt} = \left[\frac{F_{b(x)} (T_{b(x-\Delta x)} - T_{b(x)})}{t_f W \Delta x} \right] - \left[\frac{J_{w(x)} (T_{b(x)} - T_{p(x)})}{t_f} \right] \quad (5.106)$$

$$\frac{dT_{p(x)}}{dt} = \left[\frac{J_{w(x)} (T_{b(x)} - T_{p(x)})}{t_f} \right] \quad (5.107)$$

T_b and T_p ($^{\circ}\text{C}$) are the temperature at retentate and permeate channels respectively. The values of average solute rejection (Sundaramoorthy et al., 2011a), total recovery and permeate flow rate at each point, and overall permeate flow rate values are calculated as:

$$\text{Rej}_{(av)} = \frac{C_{b(x=L)} - C_{p(av)}}{C_{b(x=L)}} \times 100 \quad (5.108)$$

$C_{b(x=L)}$ and $C_{p(av)}$ are the retentate and average permeate concentrations respectively.

$$C_{p(av)} = \frac{\sum C_{p(x)}}{\text{n.sub-divisions}} \quad (x = 0 \text{ to } x = L) \quad (5.109)$$

$$\text{Rec}_{(\text{Total})} = \frac{F_{p(\text{Total})}}{F_{b(0)}} \times 100 \quad (5.110)$$

$$F_{p(x)} = J_{w(x)} W \Delta x \quad (5.111)$$

$$F_{p(\text{Total})} = \sum F_{p(x)} \dots\dots\dots (x = 0 \text{ to } x = L) \quad (5.112)$$

$\text{Rec}_{(\text{Total})}$ is the total recovery rate of the whole unit.

5.6.7.2.2 The Conservation Equations of Steady State Model

The feed and permeate concentration are provided by eliminating the hold-up term in the dynamic model with re-arrangement yields the following:

$$\frac{d \left(\frac{C_{b(x)} F_{b(x)}}{t_f W} \right)}{dx} = - \frac{J_{s(x)}}{t_f} + \frac{d}{dx} \left(D_{b(x)} \frac{dC_{b(x)}}{dx} \right) \quad (5.113)$$

$$\frac{d \left(\frac{C_{p(x)} F_{p(x)}}{t_p W} \right)}{dx} = \frac{J_{s(x)}}{t_f} + \frac{d}{dx} \left(D_{p(x)} \frac{dC_{p(x)}}{dx} \right) \quad (5.114)$$

Also, the energy balance equations (assuming a constant heat capacity for permeate and brine) for the brine channel can be written as:

$$F_{b(x)} (T_{b(x-\Delta x)} - T_{b(x)}) = J_{w(x)} (T_{b(x)} - T_{p(x)}) W \Delta x \quad (5.115)$$

$$(T_{b(x)} - T_{p(x)}) = 0 \quad (5.116)$$

Al-Obaidi and Mujtaba (2016) considered the variation of the physical properties with the length of feed and permeate channels (ninth assumption). This is due to considering the variation of operating conditions with respect to the x-axis.

The proposed correlations of Koroneos et al. (2007) have been used to calculate the physical properties of the diffusion coefficient, viscosity, and density at any point along the two sides of membrane length as follows;

$$D_{b(x)} = 6.725 \times 10^{-6} \exp \left\{ 0.1546 \times 10^{-3} (C_{b(x)} \times 18.0125) - \frac{2513}{T_{b(x)} + 273.15} \right\} \quad (5.117)$$

$$D_{p(x)} = 6.725 \times 10^{-6} \exp \left\{ 0.1546 \times 10^{-3} (C_{p(x)} \times 18.0125) - \frac{2513}{T_{p(x)} + 273.15} \right\} \quad (5.118)$$

$$\mu_{b(x)} = 1.234 \times 10^{-6} \exp \left\{ \left(0.0212 C_{b(x)} \times 18.0153 \right) + \frac{1965}{T_{b(x)} + 273.15} \right\} \quad (5.119)$$

$$\mu_{p(x)} = 1.234 \times 10^{-6} \exp \left\{ \left(0.0212 C_{p(x)} \times 18.0153 \right) + \frac{1965}{T_{p(x)} + 273.15} \right\} \quad (5.120)$$

$$\rho_{b(x)} = 498.4 m_{f(x)} + \sqrt{[248400 m_{f(x)}^2 + 752.4 m_{f(x)} C_{b(x)} \times 18.0153]} \quad (5.121)$$

$$\rho_{p(x)} = 498.4 m_{p(x)} + \sqrt{[248400 m_{p(x)}^2 + 752.4 m_{p(x)} C_{p(x)} \times 18.0153]} \quad (5.122)$$

$$m_{f(x)} = 1.0069 - 2.757 \times 10^{-4} T_{b(x)} \quad (5.123)$$

$$m_{p(x)} = 1.0069 - 2.757 \times 10^{-4} T_{p(x)} \quad (5.124)$$

5.6.7.3 Model Validation

This was carried out using the experimental data of Sundaramoorthy et al. (2011b) from a laboratory-scale spiral wound RO process for the removal of chlorophenol from wastewater. Tables 5.10, 5.11, and 5.12 compare the experimental results of chlorophenol removal and the model prediction for several operating parameters and process performance with different feed flow rates, pressures, and concentrations. As can be seen, the predicted values of the theoretical model are in good agreement with experimental ones over the ranges of pressure and concentration. The model tends to underestimate the outlet permeate concentration only for lower values of

TABLE 5.10
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(i)} = 2.166E-4 \text{ m}^3/\text{s}$)

Exp No	$P_{b(i)}$, atm	$C_{b(i)}$, E+3 (kmol/m ³)	$T_{b(i)}$, °C	$C_{b(i)}$, E+3 (kmol/m ³)		%Error	$C_{p(a)}$, E+3 (kmol/m ³)		%Error	$\% \text{ Rej}_{sw}$		%Error	$F_{b(i)}$, E+4 (m ³ /s)		%Error
				Exp.	Model		Exp.	Model		Exp.	Model		Exp.	Model	
1	5.83	0.778	30	0.854	0.850	0.50	0.370	0.390	-6.21	56.7	53.76	5.18	1.80	1.88	-4.88
2	7.77	0.778	30	0.904	0.901	0.35	0.368	0.375	-2.14	59.3	57.8	2.52	1.67	1.75	-5.02
3	9.71	0.778	30	0.948	0.935	1.33	0.366	0.375	-2.45	61.4	59.89	2.45	1.59	1.62	-1.88
4	11.64	0.778	30	1.002	0.983	1.96	0.363	0.381	-5.04	63.8	61.24	4.01	1.50	1.48	0.73
5	13.58	0.778	30	1.065	1.036	2.73	0.36	0.391	-8.61	66.2	62.27	5.93	1.37	1.35	0.94
6	5.83	1.556	32	1.711	1.723	-0.68	0.652	0.696	-6.74	61.9	59.57	3.76	1.906	1.89	0.52
7	7.77	1.556	32	1.778	1.823	-2.50	0.642	0.635	1.09	63.9	65.18	-2.00	1.736	1.76	-1.61
8	9.71	1.556	32	1.850	1.936	-4.62	0.631	0.613	2.85	65.9	68.34	-3.70	1.63	1.63	-0.14
9	11.64	1.556	32	1.943	2.064	-6.17	0.624	0.608	2.46	67.9	70.51	-3.84	1.523	1.50	1.33
10	13.58	1.556	32	2.050	2.209	-7.75	0.615	0.613	0.22	70.0	72.22	-3.17	1.416	1.37	2.98
11	5.83	2.335	32	2.575	2.58	-0.17	0.886	0.94	-6.09	65.6	63.25	3.58	1.868	1.90	-2.03
12	7.77	2.335	32	2.662	2.73	-2.53	0.884	0.852	3.619	66.8	68.81	-3.00	1.761	1.77	-0.90
13	9.71	2.335	32	2.791	2.9	-3.90	0.882	0.814	7.70	68.4	71.95	-5.19	1.666	1.64	1.02
14	11.64	2.335	32	2.894	3.09	-6.74	0.880	0.801	8.97	69.6	74.11	-6.47	1.566	1.52	2.74
15	13.58	2.335	32	3.044	3.31	-8.70	0.880	0.802	8.86	71.1	75.78	-6.58	1.478	1.39	5.41
16	5.83	3.891	32	4.245	4.268	-0.54	1.244	1.180	5.14	70.7	72.35	-2.33	1.898	1.92	-1.42
17	7.77	3.891	32	4.444	4.525	-1.82	1.231	1.240	-0.73	72.3	72.59	-0.40	1.808	1.80	0.44
18	9.71	3.891	32	4.590	4.801	-4.59	1.299	1.170	9.93	71.7	75.68	-5.55	1.681	1.67	0.23
19	11.64	3.891	32	4.753	5.111	-7.51	1.198	1.140	4.84	74.8	77.78	-3.98	1.65	1.55	5.63
20	13.58	3.891	32	5.029	5.460	-8.55	1.187	1.126	5.13	76.4	79.38	-3.90	1.536	1.43	6.44
21	5.83	6.226	31	6.800	6.750	0.85	1.668	1.82	-9.11	75.5	73.08	3.20	1.923	1.95	-1.47
22	7.77	6.226	31	7.111	7.105	0.09	1.657	1.59	4.04	76.7	77.55	-0.31	1.828	1.83	-0.54
23	9.71	6.226	31	7.381	7.495	-1.54	1.491	1.495	-0.26	79.8	80.05	-0.31	1.75	1.72	1.37
24	11.64	6.226	31	7.763	7.928	-2.12	1.475	1.451	1.62	81.0	81.69	-0.85	1.641	1.61	1.58
25	13.58	6.226	31	8.049	8.411	-4.48	1.457	1.436	1.44	81.9	82.92	-1.24	1.575	1.50	4.38

(Adapted from Al-Obaidi and Mujiaba, 2016)

TABLE 5.11
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(0)} = 2.33E-4 \text{ m}^3/\text{s}$)

Exp No	$P_{b(0)}$ atm	$C_{b(0)}$ (kmol/m ³)	$T_{b(0)}$ °C	$C_{b(L)}$ (kmol/m ³)		%Error	$C_{p(av)}$ (kmol/m ³)		%Error	% Rej _{av}		%Error	$F_{b(L)}$ (m ³ /s)		%Error
				Exp.	Model		Exp.	Model		Exp.	Model		Exp.	Model	
1	5.83	0.778	30	0.856	0.84	1.42	0.375	0.39	-4.80	56.2	53.4	4.98	1.957	2.05	-5.10
2	7.77	0.778	30	0.890	0.88	0.92	0.373	0.37	0.32	58.1	57.8	0.46	1.86	1.92	-3.33
3	9.71	0.778	30	0.937	0.92	1.49	0.372	0.37	0.88	60.3	60.0	0.43	1.742	1.78	-2.64
4	11.64	0.778	30	0.984	0.97	1.73	0.37	0.37	-0.81	62.4	61.4	1.58	1.639	1.65	-0.97
5	13.58	0.778	30	1.033	1.01	1.91	0.367	0.38	-3.89	64.5	62.4	3.22	1.542	1.52	1.16
6	5.83	1.556	32	1.703	1.71	-0.26	0.632	0.70	-10.44	62.9	59.1	6.02	2.01	2.06	-2.63
7	7.77	1.556	32	1.765	1.80	-1.95	0.625	0.63	-0.48	64.6	65.1	-0.78	1.894	1.93	-1.90
8	9.71	1.556	32	1.839	1.90	-3.46	0.618	0.60	2.63	66.4	68.4	-2.99	1.794	1.79	-0.27
9	11.64	1.556	32	1.926	2.02	-4.73	0.605	0.59	1.85	68.6	70.6	-2.88	1.684	1.66	0.95
10	13.58	1.556	32	2.023	2.15	-6.14	0.599	0.60	0.66	70.4	72.3	-2.64	1.594	1.53	3.51
11	5.83	2.335	31	2.568	2.54	1.11	0.804	0.85	-6.09	68.7	66.5	3.27	2.022	2.07	-2.81
12	7.77	2.335	31	2.673	2.67	0.12	0.802	0.76	5.23	70.0	71.4	-1.92	1.907	1.95	-2.35
13	9.71	2.335	31	2.783	2.82	-1.14	0.796	0.73	8.04	71.4	74.0	-3.61	1.815	1.82	-0.60
14	11.64	2.335	31	2.900	2.97	-2.50	0.786	0.72	8.14	72.9	75.7	-3.84	1.707	1.70	0.29
15	13.58	2.335	31	3.035	3.15	-3.78	0.777	0.73	6.69	74.4	77.0	-3.45	1.591	1.57	0.75
16	5.83	6.226	31	6.768	6.71	0.86	1.726	1.82	-5.44	74.5	72.8	2.33	2.082	2.11	-1.68
17	7.77	6.226	31	7.029	7.03	0.00	1.645	1.58	3.82	76.6	77.2	-0.84	1.987	2.00	-0.85
18	9.71	6.226	31	7.287	7.39	-1.43	1.472	1.47	0.06	79.8	80.1	-0.37	1.902	1.89	0.63
19	11.64	6.226	31	7.622	7.79	-2.16	1.433	1.42	1.04	81.2	81.8	-0.72	1.815	1.77	2.03
20	13.58	6.226	31	7.971	8.23	-3.17	1.419	1.40	1.69	82.2	83.0	-0.99	1.734	1.66	3.86

(Adapted from Al-Obaidi and Mujtaba, 2016)

TABLE 5.12
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(0)} = 2.583E-4 \text{ m}^3/\text{s}$)

Exp No	$P_{b(0)}$, atm	$C_{b(0)}$ E+3 (kmol/m ³)	$T_{b(0)}$ °C	$C_{b(0)}$ E+3 (kmol/m ³)		%Error	$C_{p(av)}$ E+3 (kmol/m ³)		%Error	% Rej _{av}		%Error	$F_{b(t)}$ E+4 (m ³ /s)		%Error
				Exp.	Model		Exp.	Model		Exp.	Model		Exp.	Model	
1	5.83	0.778	29.5	0.850	0.84	1.84	0.359	0.41	-13.37	57.8	51.21	11.40	2.2	2.31	-5.31
2	7.77	0.778	29.5	0.893	0.87	2.95	0.352	0.38	-8.12	60.6	56.14	7.35	2.075	2.18	-5.15
3	9.71	0.778	29.5	0.932	0.90	3.21	0.347	0.38	-8.06	62.8	58.44	6.94	1.953	2.04	-4.86
4	11.64	0.778	29.5	0.960	0.94	2.17	0.343	0.38	-10.11	64.3	59.8	6.99	1.838	1.91	-4.18
5	13.58	0.778	29.5	1.008	0.98	2.91	0.34	0.38	-12.94	66.3	60.74	8.38	1.72	1.78	-3.66
6	5.83	1.556	31	1.698	1.68	1.07	0.591	0.63	-7.27	65.2	62.25	4.52	2.262	2.32	-2.87
7	7.77	1.556	31	1.76	1.76	0.22	0.572	0.56	1.39	67.5	66.86	0.94	2.148	2.19	-2.23
8	9.71	1.556	31	1.825	1.84	-0.76	0.553	0.54	2.53	69.7	70.67	-1.39	2.042	2.06	-1.14
9	11.64	1.556	31	1.909	1.93	-1.06	0.55	0.53	3.25	71.2	72.43	-1.72	1.947	1.93	0.56
10	13.58	1.556	31	1.996	2.03	-1.73	0.549	0.53	2.73	72.5	73.7	-1.65	1.85	1.80	2.32
11	5.83	2.335	31	2.548	2.52	1.18	0.767	0.86	-12.51	69.9	65.73	5.96	2.29	2.33	-2.052
12	7.77	2.335	31	2.657	2.63	0.91	0.752	0.76	-0.69	71.7	71.24	0.64	2.173	2.20	-1.69
13	9.71	2.335	31	2.735	2.76	-0.87	0.744	0.72	3.83	72.8	74.07	-1.74	2.08	2.08	-0.14
14	11.64	2.335	31	2.841	2.90	-2.00	0.733	0.70	4.54	74.2	75.85	-2.22	1.97	1.95	0.65
15	13.58	2.335	31	2.987	3.05	-2.12	0.726	0.70	3.99	75.7	77.15	-1.91	1.868	1.83	1.87
16	5.83	3.891	32	xx	4.20	xx	xx	1.43	xx	xx	65.98	xx	xx	2.34	xx
17	7.77	3.891	32	xx	4.40	xx	xx	1.22	xx	xx	72.33	xx	xx	2.22	xx
18	9.71	3.891	32	4.504	4.63	-2.68	1.126	1.12	0.26	75	75.71	-0.94	2.113	2.09	0.66
19	11.64	3.891	32	4.635	4.87	-5.02	1.108	1.08	2.88	76.1	77.90	-2.36	2.07	1.97	4.54
20	13.58	3.891	32	4.831	5.14	-6.39	1.092	1.05	3.47	77.4	79.50	-2.71	1.972	1.85	5.98
21	5.83	6.226	31	6.733	6.66	1.16	1.845	1.85	-0.48	72.6	72.15	0.61	2.337	2.37	-1.60
22	7.77	6.226	31	6.977	6.94	0.49	1.549	1.57	-1.35	77.8	77.38	0.53	2.253	2.26	-0.31
23	9.71	6.226	31	7.213	7.26	-0.65	1.486	1.44	3.02	79.4	80.14	-0.93	2.17	2.14	1.15
24	11.64	6.226	31	7.497	7.61	-1.47	1.387	1.38	0.72	81.5	81.90	-0.49	2.09	2.03	2.78
25	13.58	6.226	31	7.794	7.99	-2.52	1.325	1.35	-1.50	83	83.17	-0.20	2.012	1.91	4.67

Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi and Mujtaba, 2016)

inlet concentration. This may possibly be attributed to negligible bulk flow in the spiral direction of the unit.

5.6.8 MODEL VIII: AL-OBAYDI ET AL. (2017B)

The literature shows that the models previously developed are restricted to a one-dimensional spiral wound RO process model used especially for wastewater treatment and which did not take into consideration the tangential directional impact. In most published literature, the feed flow rate is in the axial direction while the permeate flow rate is in the spiral direction. Current models do not appear to consider the impact of tangential feed flow rate and axial permeate flow rate due the underlying turbulence. Furthermore, high pressures create substantial variation in the fluid mixing, mass transfer coefficient, and pressure drop. To this extent, Al-Obaydi et al. (2017b) developed a two-dimensional mathematical (steady state and dynamic) model for a dilute aqueous solution in a spiral wound RO system. This model is considered as an extension of the Al-Obaydi and Mujtaba (2016) model, as it takes into account the variation of operating parameters along the two axes of the membrane.

Note that the assumptions made for Al-Obaydi and Mujtaba's (2016) model are valid for the Al-Obaydi et al. (2017b) model, except for considering the variation of operating parameters along both the x and y axes and relaxing a constant permeate pressure at the permeate channel (1 atm). However, the following two reasonable assumptions were used to develop this model:

- The average value of the permeate concentration for all the increments in two dimensions is taken as the total permeate concentration.
- The physical properties vary along the two dimensions (x and y) of the feed and permeate channels.

5.6.8.1 Model Equations

The dynamic axial and vertical water and solute fluxes are represented as:

$$\frac{dJ_{w(x,y)}}{dt} = \left\{ \left(A_w \left((P_{b(x,y)} - P_{p(x,y)}) - RT_{b(x,y)} (C_{w(x,y)} - C_{p(x,y)}) \right) \right) - J_{w(x,y)} \right\} \left(\frac{F_{b(x,y)}}{t_f \Delta x \Delta y} \right) \quad (5.125)$$

$$\frac{dJ_{s(x,y)}}{dt} = \left\{ \left(B_s \exp \left(\frac{J_{w(x,y)}}{k_{(x,y)}} \right) (C_{b(x,y)} - C_{p(x,y)}) \right) - J_{s(x,y)} \right\} \left(\frac{F_{b(x,y)}}{t_f \Delta x \Delta y} \right) \quad (5.126)$$

The dynamic axial and vertical membrane wall concentration is:

$$\frac{dC_{w(x,y)}}{dt} = \left\{ \left(C_{p(x,y)} + \exp\left(\frac{J_{w(x,y)}}{k_{(x,y)}}\right) \left(C_{b(x,y)} - C_{p(x,y)} \right) \right) - C_{w(x,y)} \right\} \left(\frac{F_{b(x,y)}}{t_f \Delta x \Delta y} \right) \quad (5.127)$$

The pressure difference and dynamic axial and vertical feed pressure and permeate pressure in both axes are given as:

$$\Delta P_{b(x,y)} = \left(P_{b(x,y)} - P_{p(x,y)} \right) \quad (5.128)$$

$$\begin{aligned} \frac{dP_{b(x,y)}}{dt} = & \left[\left[\left((-b F_{b(x,y)}) \right) \left(\frac{F_{b(x,y)}}{\Delta x t_f} \right) \right] - \left[\left(\frac{dP_{b(x,y)}}{dx} \right) \left(\frac{F_{b(x,y)}}{\Delta y t_f} \right) \right] \right. \\ & \left. - \left[\left(\frac{dP_{b(x,y)}}{dy} \right) \left(\frac{F_{b(x,y)}}{\Delta x t_f} \right) \right] \right] \end{aligned} \quad (5.129)$$

$$\begin{aligned} \frac{dP_{p(x,y)}}{dt} = & \left[\left[\left((-b F_{p(x,y)}) \right) \left(\frac{F_{p(x,y)}}{\Delta y t_p} + \frac{F_{p(x,y)}}{\Delta x t_p} \right) \right] - \left[\left(\frac{dP_{p(x,y)}}{dx} \right) \left(\frac{F_{p(x,y)}}{\Delta y t_p} \right) \right] \right. \\ & \left. - \left[\left(\frac{dP_{p(x,y)}}{dy} \right) \left(\frac{F_{p(x,y)}}{\Delta x t_p} \right) \right] \right] \end{aligned} \quad (5.130)$$

The dynamic axial and vertical feed flow rate and permeate flow rate are calculated from:

$$\begin{aligned} \frac{dF_{b(x,y)}}{dt} = & \left\{ \left[-(\Delta y) \left(J_{w(x,y)} \right) \right] - \left(\frac{dF_{b(x,y)}}{dx} \right) \right\} \left\{ \frac{F_{b(x,y)}}{t_f \Delta y} \right\} \\ & + \left\{ \left[-(\Delta x) \left(J_{w(x,y)} \right) \right] - \left(\frac{dF_{b(x,y)}}{dy} \right) \right\} \left\{ \frac{F_{b(x,y)}}{t_f \Delta x} \right\} \end{aligned} \quad (5.131)$$

$$F_{p(x,y)} = J_{w(x,y)} \Delta x \Delta y \quad (5.132)$$

The dynamic variation of axial and vertical feed and permeate concentrations are:

$$\begin{aligned} \frac{dC_{b(x,y)}}{dt} = & -\frac{C_{b(x,y)}}{t_f \Delta y} \frac{dF_{b(x,y)}}{dx} - \frac{F_{b(x,y)}}{t_f \Delta y} \frac{dC_{b(x,y)}}{dx} + \frac{d}{dx} \left[Db(x,y) \frac{dC_{b(x,y)}}{dx} \right] \\ & -\frac{C_{b(x,y)}}{t_f \Delta x} \frac{dF_{b(x,y)}}{dy} - \frac{F_{b(x,y)}}{t_f \Delta x} \frac{dC_{b(x,y)}}{dy} + \frac{d}{dy} \left[Db(x,y) \frac{dC_{b(x,y)}}{dy} \right] \\ & + \frac{J_{s(x,y)}}{t_f} \end{aligned} \quad (5.133)$$

$$\begin{aligned} \frac{dC_{p(x,y)}}{dt} = & -\frac{C_{p(x,y)}}{t_f \Delta y} \frac{dF_{p(x,y)}}{dx} - \frac{F_{p(x,y)}}{t_f \Delta y} \frac{dC_{p(x,y)}}{dx} \\ & + \frac{d}{dx} \left[D_{p(x,y)} \frac{dC_{p(x,y)}}{dx} \right] - \frac{C_{p(x,y)}}{t_f \Delta x} \frac{dF_{p(x,y)}}{dy} \\ & - \frac{F_{p(x,y)}}{t_f \Delta x} \frac{dC_{p(x,y)}}{dy} + \frac{d}{dy} \left[D_{p(x,y)} \frac{dC_{p(x,y)}}{dy} \right] + \frac{J_{s(x,y)}}{t_f} \end{aligned} \quad (5.134)$$

Eq. (5.135) is used to calculate the average value of permeate concentration, which is then used to calculate the average solute rejection, as follows:

$$C_{p(av)} = \frac{\sum C_{p(x,y)}}{\text{n.sub-divisions}} \quad (5.135)$$

$$\text{Rej}_{(av)} = \frac{C_{b(x=L,y)} - C_{p(av)}}{C_{b(x=L,y)}} \times 100 \quad (5.136)$$

The dynamic axial and vertical feed and permeate temperatures are:

$$\begin{aligned} \frac{dT_{b(x,y)}}{dt} = & \left[\frac{F_{b(x,y)} (T_{b(x-1,y)} - T_{b(x,y)})}{t_f \Delta x \Delta y} \right] \\ & - \left[\frac{J_{w(x,y)} (T_{b(x,y)} - T_{p(x,y)})}{t_f} \right] \end{aligned} \quad (5.137)$$

$$\frac{dT_{p(x,y)}}{dt} = \left[\frac{J_{w(x,y)} (T_{b(x,y)} - T_{p(x,y)})}{t_f} \right] \quad (5.138)$$

The total permeate flow rate in the permeate channel is calculated as the summation of permeate flux of all the dimensions of axes. This is then used to calculate the total recovery (–) as follows:

$$F_{p(\text{Total})} = \sum F_{p(x,y)} \tag{5.139}$$

$$\text{Rec}_{(\text{Total})} = \frac{F_{p(\text{Total})}}{F_{b(0,y)}} \times 100 \tag{5.140}$$

The set of physical properties used by Al-Obaidi and Mujtaba (2016) is valid for the Al-Obaidi et al. (2017b) model.

5.6.8.2 Parameter Estimation

The parameters of the model were estimated using the graphical method of linear fit as applied by Sundaramoorthy et al. (2011a). The parameters include the solvent transport coefficient A_w , dimethylphenol transport coefficient B_s , and the feed channel friction parameter b . The results of parameter estimation are based on the experimental data of Srinivasan et al. (2011) and are given in Table 5.13. The estimated values of A_w and B_s parameters showed some convergence with the values suggested by Srinivasan et al. (2011).

5.6.8.3 Model Validation

The steady state version of the Al-Obaidi et al. (2017b) model was validated using the experimental data of Srinivasan et al. (2011) for the rejection of dimethylphenol as a solute in dilute aqueous solutions. Tables 5.14, 5.15, and 5.16 show a comparison between the experimental results of Srinivasan et al. (2011) and the model predictions for three groups of feed flow rates. Each group holds five different feed concentrations under five different feed pressures. The percentage error between the experimental and the model predictions are estimated for comparison purposes. Tables 5.14–5.16 and Figures 5.16 and 5.17 readily show agreement between the experimental and predicted values of outlet feed concentration and dimethylphenol rejection for the entire data set and within a 5% to 2.1% error, respectively. The only limitation is that the model can predict the permeate concentration within a

TABLE 5.13
Results of Parameter Estimation

Parameter	Estimated value	(Srinivasan et al., 2011) values
b	$9400.9 \left(\frac{\text{atm s}}{\text{m}^4} \right)$	$9400.9 \left(\frac{\text{atm s}}{\text{m}^4} \right)$
A_w	$9.42009\text{E-}7 \left(\frac{\text{m}}{\text{atm s}} \right)$	$9.7388\text{E-}7 \left(\frac{\text{m}}{\text{atm s}} \right)$
B_s (dimethylphenol)	$2.22577\text{E-}8 \left(\frac{\text{m}}{\text{s}} \right)$	$1.5876\text{E-}8 \left(\frac{\text{m}}{\text{s}} \right)$

TABLE 5.14
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(0,y)} = 2.166E-4 \text{ m}^3/\text{s}$)

Exp No	Pb (inlet) (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet) (°C)	Pb(outlet), (atm)	%Error	Cb(outlet) x10 ³ (kmol/ m ³)	%Error	Cp _{av} x10 ³ (kmol/m ³)	%Error	% Rej _{av}	%Error	Fb(outlet) x10 ⁻⁴ (m ³ /s)	%Error					
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.					
1	5.83	0.819	32.5	4.46	4.06	8.96	0.950	0.92	2.84	0.0931	0.089	4.84	0.902	0.904	-0.22	1.8	1.916	-6.44
2	7.77	0.819	32.5	6.31	6.06	3.96	1.016	0.99	2.51	0.0864	0.073	15.0	0.915	0.925	-1.19	1.67	1.786	-6.94
3	9.71	0.819	32.5	8.14	8.06	0.98	1.082	1.07	1.03	0.0790	0.066	16.2	0.927	0.938	-1.20	1.59	1.656	-4.15
4	11.64	0.819	32.5	9.98	10.05	-0.70	1.156	1.17	-0.75	0.0740	0.062	15.8	0.936	0.946	-1.13	1.5	1.528	-1.86
5	13.58	0.819	32.5	11.8	12.05	-2.11	1.256	1.28	-1.83	0.0729	0.060	17.6	0.942	0.953	-1.17	1.37	1.399	-2.11
6	5.83	1.637	31	4.41	4.05	8.16	1.883	1.83	2.86	0.1526	0.173	-13.3	0.919	0.905	1.51	1.851	1.932	-4.37
7	7.77	1.637	31	6.27	6.05	3.50	2.022	1.96	3.20	0.1335	0.141	-5.24	0.934	0.927	0.68	1.736	1.807	-4.08
8	9.71	1.637	31	8.09	8.05	0.49	2.121	2.11	0.52	0.1209	0.127	-5.21	0.943	0.939	0.34	1.63	1.681	-3.12
9	11.64	1.637	31	9.93	10.03	-1.00	2.288	2.28	0.22	0.1167	0.119	-1.88	0.949	0.947	0.11	1.523	1.557	-2.23
10	13.58	1.637	31	11.76	12.03	-2.29	2.425	2.49	-2.82	0.1140	0.114	0.00	0.953	0.954	-0.13	1.416	1.433	-1.20
11	5.83	2.455	31	4.37	4.04	7.50	2.798	2.73	2.42	0.2575	0.237	8.07	0.908	0.913	-0.58	1.868	1.942	-3.96
12	7.77	2.455	31	6.22	6.04	2.92	2.978	2.92	2.06	0.2204	0.190	13.7	0.926	0.934	-0.95	1.761	1.819	-3.29
13	9.71	2.455	31	8.05	8.03	0.19	3.119	3.14	-0.50	0.1778	0.168	5.51	0.943	0.946	-0.36	1.666	1.696	-1.80
14	11.64	2.455	31	9.89	10.02	-1.31	3.352	3.39	-1.04	0.1710	0.156	8.94	0.949	0.954	-0.52	1.566	1.576	-0.63
15	13.58	2.455	31	11.72	12.02	-2.52	3.506	3.69	-5.24	0.1683	0.148	11.9	0.952	0.959	-0.81	1.478	1.453	1.69
16	5.83	4.092	30	4.32	4.03	6.71	4.660	4.51	3.28	0.3029	0.273	9.87	0.935	0.939	-0.45	1.898	1.962	-3.37
17	7.77	4.092	30	6.17	6.024	2.36	4.806	4.79	0.40	0.2884	0.313	-8.52	0.94	0.934	0.59	1.808	1.848	-2.21
18	9.71	4.092	30	8	8.017	-0.21	5.147	5.12	0.60	0.2625	0.274	-4.38	0.949	0.946	0.24	1.681	1.731	-2.97

(Continued)

TABLE 5.14
(Continued)

TABLE 5.14 (Continued)																		
Exp No	Pb (inlet) (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet) (°C)	Pb(outlet), (atm)	%Error	Cb(outlet) x10 ³ (kmol/ m ³)	%Error	Cp _{av} x10 ³ (kmol/m ³)	%Error	% Rej _{av}	%Error	Fb(outlet) x10 ⁻⁴ (m ³ /s)	%Error					
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.					
19	11.64	4.092	30	9.84	10	-1.62	5.293	5.49	-3.80	0.2382	0.253	-6.00	0.955	0.954	0.10	1.65	1.617	2.00
20	13.58	4.092	30	11.67	11.99	-2.74	5.664	5.94	-4.87	0.2096	0.238	-13.5	0.963	0.959	0.34	1.536	1.502	2.21
21	5.83	6.548	31.5	xx	4.025	xx	xx	7.16	xx	xx	0.514	xx	xx	0.928	xx	xx	1.978	xx
22	7.77	6.548	31.5	6.13	6.02	1.84	7.758	7.61	1.96	0.3724	0.388	-4.13	0.952	0.949	0.31	1.828	1.863	-1.91
23	9.71	6.548	31.5	7.96	8.01	-0.62	8.105	8.12	-0.20	0.3080	0.329	-7.11	0.962	0.959	0.28	1.75	1.747	0.17
24	11.64	6.548	31.5	9.79	9.99	-2.07	8.656	8.72	-0.68	0.2597	0.297	-14.3	0.97	0.965	0.42	1.641	1.633	0.48
25	13.58	6.548	31.5	11.62	11.98	-3.09	8.911	9.41	-5.60	0.2406	0.276	-14.7	0.973	0.970	0.24	1.575	1.517	3.68

Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi et al., 2017b)

Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi et al., 2017b)

TABLE 5.15
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(0,y)} = 2.33E-4 \text{ m}^3/\text{s}$)

No	Pb(inlet), (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet), (°C)	Pb(outlet), (atm)	%Error	Cb(outlet) x10 ³ (kmol/ m ³)	%Error	Cp _{av} x10 ³ (kmol/m ³)	%Error	% Rej _{av}	%Error	Fb(outlet) x10 ⁴ (m ³ /s)	%Error					
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.					
1	5.83	0.819	32.5	4.39	3.92	10.7	0.943	0.912	3.24	0.091	0.088	3.06	0.903	0.902	0.02	1.957	2.085	-6.54
2	7.77	0.819	32.5	6.23	5.92	5.04	1.005	0.974	3.16	0.085	0.072	15.4	0.915	0.925	-1.16	1.86	1.955	-5.10
3	9.71	0.819	32.5	8.06	7.92	1.78	1.060	1.045	1.41	0.074	0.064	12.8	0.93	0.938	-0.87	1.742	1.825	-4.76
4	11.64	0.819	32.5	9.9	9.91	-0.07	1.124	1.130	-0.47	0.073	0.060	17.2	0.935	0.946	-1.22	1.639	1.694	-3.35
5	13.58	0.819	32.5	11.73	11.91	-1.51	1.196	1.228	-2.66	0.062	0.058	6.75	0.948	0.952	-0.49	1.542	1.566	-1.55
6	5.83	1.637	31	4.34	3.91	9.90	1.875	1.811	3.41	0.151	0.173	-13.8	0.919	0.904	1.63	2.01	2.1	-4.47
7	7.77	1.637	31	6.19	5.89	4.70	1.983	1.928	2.77	0.128	0.139	-7.83	0.935	0.927	0.81	1.894	1.975	-4.31
8	9.71	1.637	31	8.02	7.91	1.43	2.092	2.062	1.48	0.119	0.124	-3.93	0.943	0.939	0.34	1.794	1.848	-3.01
9	11.64	1.637	31	9.86	9.89	-0.30	2.201	2.217	-0.68	0.112	0.115	-2.40	0.949	0.947	0.12	1.684	1.723	-2.31
10	13.58	1.637	31	11.68	11.88	-1.71	2.361	2.400	-1.62	0.111	0.110	0.63	0.953	0.954	-0.10	1.594	1.598	-0.30
11	5.83	2.455	31	4.29	3.89	9.13	2.773	2.706	2.43	0.230	0.237	-2.95	0.917	0.912	0.51	2.022	2.109	-4.30
12	7.77	2.455	31	6.14	5.89	4.00	2.951	2.875	2.58	0.212	0.187	11.8	0.928	0.934	-0.73	1.907	1.986	-4.14
13	9.71	2.455	31	7.97	7.89	1.00	3.100	3.070	0.96	0.173	0.164	5.24	0.944	0.946	-0.25	1.815	1.863	-2.64
14	11.64	2.455	31	9.81	9.88	-0.67	3.280	3.294	-0.42	0.164	0.151	7.62	0.95	0.954	-0.42	1.707	1.74	-1.93
15	13.58	2.455	31	11.64	11.88	-2.06	3.502	3.558	-1.59	0.154	0.143	6.87	0.956	0.959	-0.37	1.591	1.618	-1.69
16	5.83	4.092	30	4.25	3.89	8.54	4.554	4.468	1.90	0.291	0.277	4.97	0.936	0.938	-0.21	2.072	2.129	-2.75
17	7.77	4.092	30	6.10	5.88	3.60	4.796	4.724	1.51	0.273	0.310	-13.3	0.943	0.934	0.92	1.974	2.015	-2.07
18	9.71	4.092	30	7.92	7.87	0.63	4.993	5.02	-0.56	0.244	0.269	-9.93	0.951	0.946	0.48	1.887	1.897	-0.52

(Continued)

TABLE 5.15
(Continued)

TABLE 5.15 (Continued)																		
No	Pb(inlet), (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet), (°C)	Pb(outlet), (atm)	%Error	Cb(outlet) x10 ³ (kmol/ m ³)	%Error	Cp _{av} x10 ³ (kmol/m ³)	%Error	% Rej _{av}	%Error	Fb(outlet) x10 ⁴ (m ³ /s)	%Error					
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.					
19	11.64	4.092	30	9.76	9.85	-0.92	5.179	5.361	-3.51	0.222	0.246	-10.4	0.957	0.954	0.30	1.805	1.783	1.21
20	13.58	4.092	30	11.59	11.85	-2.24	5.436	5.755	-5.86	0.195	0.231	-18.0	0.964	0.959	0.44	1.722	1.664	3.36
21	5.83	6.548	31.5	xx	3.88	xx	xx	7.104	xx	0.519	xx	xx	xx	0.926	xx	xx	2.144	xx
22	7.77	6.548	31.5	6.05	5.87	2.92	7.555	7.510	0.59	0.355	0.384	-8.25	0.953	0.948	0.44	1.987	2.029	-2.11
23	9.71	6.548	31.5	7.88	7.87	0.12	7.813	7.997	-2.36	0.296	0.324	-9.12	0.962	0.959	0.28	1.902	1.913	-0.57
24	11.64	6.548	31.5	9.72	9.85	-1.33	8.180	8.510	-4.02	0.253	0.290	-14.3	0.969	0.965	0.31	1.815	1.798	0.93
25	13.58	6.548	31.5	11.54	11.84	-2.59	8.674	9.126	-5.21	0.234	0.268	-14.4	0.973	0.970	0.25	1.734	1.681	3.05

(Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi et al., 2017b)

Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi et al., 2017b)

TABLE 5.16
The Model Validation with Experimental Results for Inlet Feed Flow Rate of ($F_{b(0,y)} = 2.583E-4 \text{ m}^3/\text{s}$)

No	Pb (inlet) (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet) (°C)	Pb(outlet), (atm)		%Error	Cb(outlet)x10 ³ (kmol/m ³)		%Error	Cp _{av} x10 ³ (kmol/m ³)		%Error	% Rej _{av}		%Error	Fb(outlet)x10 ⁴ (m ³ /s)	%Error	
				Exp.	The.		Exp.	The.		Exp.	The.		Exp.	The.		Exp.	The.	
1	5.83	0.819	32.5	4.27	3.69	13.5	0.929	0.899	3.15	0.086	0.089	-3.68	0.907	0.900	0.72	2.199	2.345	-6.63
2	7.77	0.819	32.5	6.11	5.69	6.87	0.997	0.953	4.43	0.079	0.071	11.0	0.92	0.925	-0.59	2.075	2.21	-6.50
3	9.71	0.819	32.5	7.94	7.69	3.14	1.061	1.016	4.24	0.062	0.062	-0.11	0.941	0.938	0.28	1.953	2.08	-6.50
4	11.64	0.819	32.5	9.78	9.67	1.12	1.116	1.084	2.86	0.055	0.058	-4.30	0.95	0.946	0.40	1.838	1.955	-6.36
5	13.58	0.819	32.5	11.61	11.68	-0.60	1.207	1.178	2.40	0.049	0.055	-11.3	0.959	0.953	0.61	1.72	1.807	-5.05
6	5.83	1.637	31	4.22	3.68	12.7	1.848	1.788	3.25	0.146	0.175	-19.8	0.921	0.901	2.10	2.261	2.359	-4.33
7	7.77	1.637	31	6.07	5.68	6.42	1.952	1.889	3.24	0.123	0.137	-11.3	0.937	0.927	1.05	2.148	2.23	-3.81
8	9.71	1.637	31	7.89	7.67	2.78	2.045	2.005	1.98	0.116	0.121	-3.77	0.943	0.939	0.36	2.042	2.107	-3.18
9	11.64	1.637	31	9.73	9.67	0.61	2.146	2.136	0.47	0.111	0.114	-2.95	0.948	0.947	0.02	1.947	1.982	-1.79
10	13.58	1.637	31	11.56	11.66	-0.86	2.220	2.288	-3.04	0.108	0.105	2.94	0.951	0.953	-0.29	1.85	1.855	-0.27
11	5.83	2.455	31	4.17	3.68	11.8	2.745	2.672	2.68	0.227	0.240	-5.30	0.917	0.91	0.76	2.29	2.368	-3.40
12	7.77	2.455	31	6.02	5.67	5.79	2.898	2.820	2.71	0.200	0.184	7.65	0.931	0.934	-0.37	2.173	2.245	-3.31
13	9.71	2.455	31	7.85	7.67	2.31	2.982	2.988	-0.19	0.167	0.160	4.07	0.944	0.946	-0.25	2.08	2.121	-1.97
14	11.64	2.455	31	9.66	9.65	0.06	3.165	3.179	-0.41	0.148	0.146	1.68	0.953	0.953	-0.09	1.97	1.997	-1.37
15	13.58	2.455	31	11.51	11.65	-1.21	3.314	3.399	-2.55	0.139	0.137	1.14	0.958	0.959	-0.15	1.868	1.874	-0.32
16	5.83	4.092	29	xx	3.66	xx	xx	4.408	xx	xx	0.316	xx	xx	0.928	xx	xx	2.393	xx
17	7.77	4.092	29	xx	5.65	xx	xx	4.630	xx	xx	0.232	xx	xx	0.949	xx	xx	2.278	xx
18	9.71	4.092	29	7.8	7.65	1.92	4.900	4.882	0.36	0.230	0.198	13.9	0.953	0.959	-0.67	2.113	2.162	-2.31
19	11.64	4.092	29	9.61	9.63	-0.20	5.047	5.164	-2.30	0.212	0.180	14.9	0.958	0.965	-0.73	2.07	2.047	1.11

(Continued)

TABLE 5.16
(Continued)

No	Pb (inlet) (atm)	Cb(inlet) x10 ³ (kmol/m ³)	Tb (inlet) (°C)	Pb(outlet), (atm)	%Error	Cb(outlet)x10 ³ (kmol/m ³)	%Error	Cp _{av} x10 ³ (kmol/m ³)	%Error	% Rej _{av}	%Error	Fb(outlet)x10 ⁴ (m ³ /s)	%Error					
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.					
20	13.58	4.092	29	11.47	11.62	-1.30	5.365	5.486	-2.24	0.187	0.169	9.58	0.965	0.969	-0.41	1.972	1.93	2.12
21	5.83	6.548	31.5	4.08	3.66	10.2	7.166	7.036	1.82	0.387	0.381	1.55	0.946	0.945	0.02	2.337	2.401	-2.73
22	7.77	6.548	31.5	5.93	5.65	4.72	7.502	7.388	1.52	0.345	0.381	-10.4	0.954	0.948	0.59	2.253	2.287	-1.50
23	9.71	6.548	31.5	7.75	7.64	1.41	7.827	7.796	0.39	0.289	0.317	-9.53	0.963	0.959	0.38	2.17	2.170	-0.01
24	11.64	6.548	31.5	9.57	9.637	-0.70	8.006	8.255	-3.10	0.248	0.281	-13.2	0.969	0.965	0.33	2.09	2.053	1.77
25	13.58	6.548	31.5	11.42	11.62	-1.75	8.503	8.778	-3.22	0.229	0.258	-12.7	0.973	0.970	0.25	2.011	1.936	3.72

Note: (xx) means the experimental data have not been reported.
(Adapted from Al-Obaidi et al., 2017b)

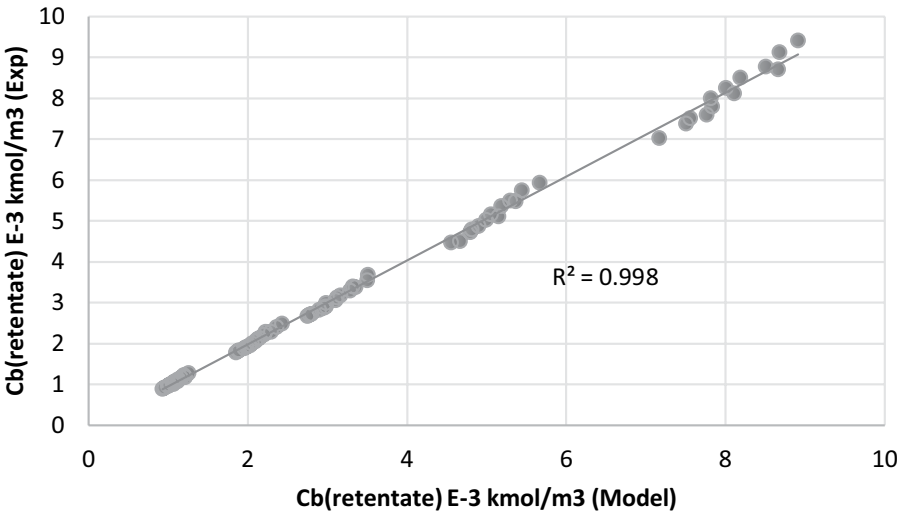


FIGURE 5.16 Comparison of experimental and model prediction of outlet brine concentration. (Adapted from Al-Obaidi et al., 2017b)

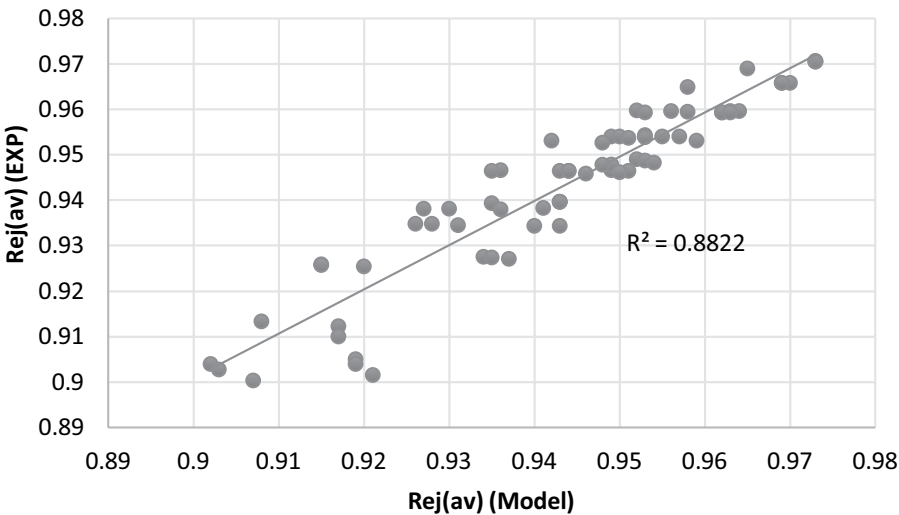


FIGURE 5.17 Comparison of experimental and model prediction of solute rejection. (Adapted from Al-Obaidi et al., 2017b)

maximum of 15% error and less than 4% error for about 76% of retentate feed flow rate readings. Finally, 79% of retentate pressure readings are within a 4% error. Therefore, one can deduce that the permeate concentration represents the parameter that causes the biggest error.

5.6.8.4 Comparison of Performances by Using Model VII and Model VIII

The model of Al-Obaidi and Mujtaba (2016), which was developed as a one-dimensional dynamic and steady state model, incorporated thermophysical properties of the dimethylphenol and the prediction of several key parameters ($Re_{j(av)}$ and $Re_{c(Total)}$) of the process. This is outlined in Table 5.17 together with the prediction of the same parameters obtained using the two-dimensional Al-Obaidi et al. (2017b) model (under steady state condition).

As can be seen from Table 5.17, the accuracy of prediction using the two-dimensional model has significantly improved compared to experimental results.

5.6.9 MODEL IX: AL-OBDAIDI ET AL. (2017c)

A one-dimensional steady state model based on a wastewater treatment spiral wound RO system was developed by Al-Obaidi et al. (2017c) based on the solution-diffusion model to simulate the transport phenomena of solute and water through the membrane. The simulation results of Al-Obaidi and Mujtaba (2016) and Al-Obaidi et al. (2017b) models confirmed the marginal variation of temperature along the two axes x and y . Al-Obaidi et al. (2017c) assumed isothermal conditions.

5.6.9.1 Assumptions

The following assumptions were made to develop the proposed process model:

- Validity of solution-diffusion model to express mass transport through the membrane.
- Fixed operating conditions along the spatial direction (y -axis).
- Fixed membrane characteristics and channel geometries.
- The pressure drop along the feed channel is represented by the friction parameter based on Darcy's law.
- Fixed atmospheric pressure along the permeate.
- Fixed solute concentration along the permeate channel. However, inlet and outlet permeate solute concentrations were used to calculate the average value.
- The underlying process is set to be isothermal.
- Negligible impact of feed spacer on the fluid patterns at the feed channel.

5.6.9.2 Model Equations

Full details of the model developed can be found in Al-Obaidi et al. (2017c). However, the associated key equations are shown below.

The water flux, feed flow rate, feed pressure, and the pressure difference between the feed and permeate channels at any point along the membrane length are estimated as follows:

$$J_{w(x)} = \theta \Delta P_{b(x)} \quad (5.141)$$

TABLE 5.17
Comparison of Al-Obaidi Et Al. (2016) and Al-Obaidi Et Al. (2017b) Models Predictions against Experimental Data of Srinivasan Et Al. (2011) for Dimethylphenol Removal from Wastewater

Exp No	C _{b(inlet)} (kmol/m ³)	P _{b(inlet)} (atm)	F _{b(inlet)} (m ³ /s)	Tb (°C)	Parameter	Exp. value (Srinivasan et al., 2011)	Al-Obaidi et al. (2016)	Error %	Al-Obaidi et al. (2017a)	Error%
1	6.548E-03	13.58	2.58E-04	31.5	Re _{j(av)}	97.3	96.537	0.783	98.019	-0.74
					C _{b(outlet)}	0.0085	0.008	-3.853	0.0087	-3.34
					Rec _(Total)	22.14	27.090	-22.33	25.641	-15.79
					F _{b(outlet)}	2.01E-4	1.90E-4	5.700	1.93E-4	3.74
2	6.548E-03	11.64	2.58E-04	31.5	Re _{j(av)}	96.9	95.941	0.989	97.717	-0.84
					C _{b(outlet)}	0.0080	0.008	-3.682	0.0082	-3.20
					Rec _(Total)	19.08	22.112	-15.854	20.807	-9.02
					F _{b(outlet)}	2.09E-4	2.02E-4	3.311	2.05E-4	1.81
3	6.548E-03	9.71	2.58E-04	31.5	Re _{j(av)}	96.3	95.044	1.303	97.268	-1.01
					C _{b(outlet)}	0.0078	0.007	-0.080	0.0078	0.31
					Rec _(Total)	15.99	17.156	-7.303	15.970	0.12
					F _{b(outlet)}	2.17E-4	2.14E-4	1.178	2.17E-4	0.04
4	6.548E-03	13.58	2.33E-04	31.5	Re _{j(av)}	97.3	96.565	0.754	98.013	-0.73
					C _{b(outlet)}	0.0086	0.009	-5.821	0.0091	-5.33
					Rec _(Total)	25.58	30.101	-17.679	28.539	-11.57
					F _{b(outlet)}	1.73E-4	1.64E-4	5.273	1.68E-4	3.06
5	6.548E-03	11.64	2.33E-04	31.5	Re _{j(av)}	96.9	95.983	0.945	97.712	-0.84
					C _{b(outlet)}	0.0081	0.008	-4.606	0.0085	-4.12
					Rec _(Total)	22.10	24.655	-11.548	23.254	-5.21
					F _{b(outlet)}	1.82E-4	1.77E-4	2.720	1.80E-4	0.98
6	6.548E-03	9.71	2.33E-04	31.5	Re _{j(av)}	96.2	95.126	1.116	97.275	-1.12
					C _{b(outlet)}	0.0078	0.008	-2.597	0.0079	-2.18
					Rec _(Total)	18.37	19.221	-4.640	17.964	2.20
					F _{b(outlet)}	1.90E-4	1.89E-4	0.730	1.91E-4	-0.58

Note: E-03 = 10⁻³
(Adapted from Al-Obaidi et al., 2018d)

$$\theta = \frac{A_w B_s}{B_s + R T_b A_w C_{p(av)}} \quad (5.142)$$

$$F_{b(x)} = \left\{ F_{b(0)} - (W \theta x \Delta P_{b(0)}) + \left(W \theta b \left(\frac{x^2}{2} \right) F_{b(0)} \right) + \left(W \theta b \left(\frac{W \theta}{b} \right)^{0.5} \left(\frac{x^2}{2} \right) (\Delta P_{b(x)} - \Delta P_{b(0)}) \right) \right\} \quad (5.143)$$

$$P_{b(x)} = \left\{ P_{b(0)} - (b \times F_{b(0)}) + \left(b W \theta \left(\frac{x^2}{2} \right) (\Delta P_{b(x)}) \right) - \left[b^2 W \theta \left(\frac{x^3}{6} \right) F_{b(0)} \right] - \left[b^2 W \theta \left(\frac{W \theta}{b} \right)^{0.5} \left(\frac{x^3}{6} \right) (\Delta P_{b(x)} - \Delta P_{b(0)}) \right] \right\} \quad (5.144)$$

$$\Delta P_{b(x)} = \Delta P_{b(0)} - (b \times F_{b(0)}) - \left[\left(\frac{W \theta}{b} \right)^{0.5} b \times (\Delta P_{b(x)} - \Delta P_{b(0)}) \right] \quad (5.145)$$

The pressure loss (atm) along the membrane length is calculated using:

$$P_{loss} = P_{b(0)} - P_{b(L)} \quad (5.146)$$

Another water flux at each point along the membrane length is also developed as:

$$J_{w(x)} = \theta \left\{ \left[\Delta P_{b(0)} - (b \times F_{b(0)}) \right] - \left[\left(\frac{W \theta}{b} \right)^{0.5} b \times (\Delta P_{b(x)} - \Delta P_{b(0)}) \right] \right\} \quad (5.147)$$

The variation of bulk concentration can be estimated from:

$$C_{b(x)} = \frac{F_{b(x-1)} (C_{b(x-1)} - C_{p(av)})}{F_{b(x)}} + C_{p(av)} \quad (5.148)$$

The average value inlet and outlet permeate concentrations is applied to calculate the permeate solute concentration:

$$C_{p(av)} = \frac{C_{p(0)} + C_{p(L)}}{2} \quad (5.149)$$

$$C_{p(0)} = \frac{B_s C_{b(0)} e^{\frac{J_{w(0)}}{k(0)}}}{J_{w(0)} + B_s e^{\frac{J_{w(0)}}{k(0)}}} \quad (5.150)$$

$$C_{p(L)} = \frac{B_s C_{b(L)} e^{\frac{J_{w(L)}}{k(L)}}}{J_{w(L)} + B_s e^{\frac{J_{w(L)}}{k(L)}}} \quad (5.151)$$

The permeate flux and bulk velocity at any point along the membrane length are:

$$F_{p(x,y)} = F_{p(0)} + \left(W \times \theta \Delta P_{b(0)} \right) - \left[W \theta b \left(\frac{x^2}{2} \right) F_{b(0)} \right] \\ - \left[W \theta b \left(\frac{x^2}{2} \right) \left(\frac{W \theta}{b} \right)^{0.5} \left(\Delta P_{b(x)} - \Delta P_{b(0)} \right) \right] \quad (5.152)$$

$$U_{b(x)} = \frac{F_{b(x)}}{t_f W} \quad (5.153)$$

5.6.9.3 Parameter Estimation Using the gPROMS Software Suite

Unknown parameters of any developed model and the operating conditions should be determined before solving the model equations. Al-Obaidi et al. (2017e) have consistently used another method to estimate these unknown parameters, which took advantage of the automated parameter estimation tool gEST available in gPROMS (Process System Enterprise Ltd., 2001) for each set of experiments. An optimisation was then used to accurately evaluate the values of several parameters depending on the best experimental information that would yield the best performance criterion. This is to minimise the sum of square errors (SSE) between the experimental values of several parameters and the calculated values. This was achieved by altering the model parameters from an initial guesstimate value to optimal values based on experimental data—this process uses what is commonly called as the optimisation solver (Jarullah et al., 2011). The gPROMS software provides a mathematical solver tool called MXLKHD, which uses the maximum likelihood optimisation method.

The methodology of parameter estimation starts with actual experimental data, which is used find the SSE between the experimental retentate concentration, average permeate concentration, retentate flow rate, total permeated water, retentate pressure, and solute rejection.

The process model equations of any distributed model developed can be written in a compact form as follows:

$$f(z, x(z), x^-(z), u(z), v) = 0; [z_0, z_f]$$

z is the independent variable (length of membrane), $x(z)$ is the set of all differential and algebraic variables, $\dot{x}(z)$ represents the derivative of $x(z)$ with respect to length of membrane, $u(z)$ is the control variables, and v denotes the constant parameters of the process. The membrane length under consideration $[z_0, z_f]$ and function f is assumed to be continuously differentiable with respect to all its arguments.

For any lumped models developed, the non-linear algebraic equations can be written in another compact form of: $f(x, u, v) = 0$, where x is the set of all algebraic variables, u is the set of decision variables need to be optimised, and v represents the constant parameters of the model.

The parameter estimation problem can be formulated as follows:

- Given: time invariant parameters: inlet feed concentration, flow rate, pressure, and temperature.
- Measured variables data: retentate measured concentration, average permeate concentration, retentate flow rate, retentate pressure, total permeated flow rate, and rejection.
- Obtain: model unknown parameters.
- Minimising: the sum of square errors.
- Subject to: process model, process constraints.

For instance, SSE for the retentate concentration is:

$$SSE = \sum_{i=1}^{N_{Data}} \left[C_{b(L)}^{Exp.} - C_{b(L)}^{Cal.} \right]^2 \quad (5.154)$$

In Eq. (5.154), N_{Data} , $C_{b(L)}^{Exp.}$, and $C_{b(L)}^{Cal.}$ are the numbers of test runs and experimental and calculated outlet feed concentration, respectively.

The complete specification of a parameter estimation problem for the model requires:

Min *SSE*

decision variables (model unknown parameters)

Subject to: Equality constraints:

Process model: $f(z, x(z), \dot{x}(z), u(z), v) = 0; [z_0, z_f]$

Inequality constraints:

lower value " decision variable1" upper value

lower value " decision variable2" upper value

A simulation step of the model solver starts the parameter estimation approach by converging the equality constraints (described by f) to satisfy the lower and upper bounds of inequality constraints of decision variables. The problem can then be solved by renewing the decision variables in a way that satisfies the equality and inequality constraints (Mujtaba, 2004).

Basically, the parameter estimation methodology of gPROMS has been used by several researchers in several industrial operations. This is formulated as a non-linear programming (NLP) problem subject to non-linear and differential-algebraic

constraints. These are solved using a successive quadratic programming (SQP) method based on the observational data for the relevant pollutant that can be found in the literature. Broadly speaking, this methodology has frequently provided local solutions and cannot guarantee global optimality with certainty (Moles et al., 2003). In other words, there is a limitation on determining high-consistent parameters compared to stochastic global optimisation methods such as stochastic algorithm and evolution strategies. However, the observed numerical convergence of the sum of square errors was investigated for these models has indicated good corroboration with satisfactory solutions.

5.6.9.3.1 Parameters Estimation Results

The model of Al-Obaidi et al. (2017c) used the experimental data of Fujioka et al. (2014) of N-nitrosamine removal from wastewater using a series of seven membrane elements to estimate the unknown parameters of the model. These experiments were carried out at the operating conditions of 6.51 atm, 2.43E-3 m³/s, 250 ppm, and 20 °C. In this respect, the gEST parameter estimation tool in the gPROMS suite was used to estimate model parameters. They included the variation of water permeability parameter and NDMA transport parameter between 1.0 and 1.22E-6 m/s atm and between 5.15 and 5.67E-6 m/s, respectively. Therefore, new equations were developed to calculate the water and NDMA transport parameters based on the inlet operating conditions. Fujioka et al. (2014) considered the values of water and NDMA transport parameters of 1.4E-6 m/s atm and 5.35E-6 m/s, respectively. Another equation to calculate the friction parameter was developed based on the average Reynolds number along the membrane length, as follows:

$$A_w = 0.3333 \left\{ \left(2E - 7 P_{b(0)} \right) + \left(0.0013 F_{b(0)} \right) - \left(785.44 C_{b(0)} \right) + 2.1E - 6 \right\} \quad (5.155)$$

$$B_s = 0.3333 \left\{ \left(3E - 7 P_{b(0)} \right) + \left(0.0023 F_{b(0)} \right) - \left(1364.6 C_{b(0)} \right) + 1.406E - 5 \right\} \quad (5.156)$$

$$b = 1.8052 Re_{(av)} - 793.46 \quad (5.157)$$

$$Re_{(x)} = \frac{2 \rho_{b(x)} t_f U_{b(x)}}{\mu_{b(x)}} \quad (5.158)$$

5.6.9.4 Model Validation

Figure 5.18 depicts the comparative analysis of several operating conditions between the experimental results and the model predictions. Overall, the model could predict the variation of the retentate pressure and water flux along the x-axis of seven

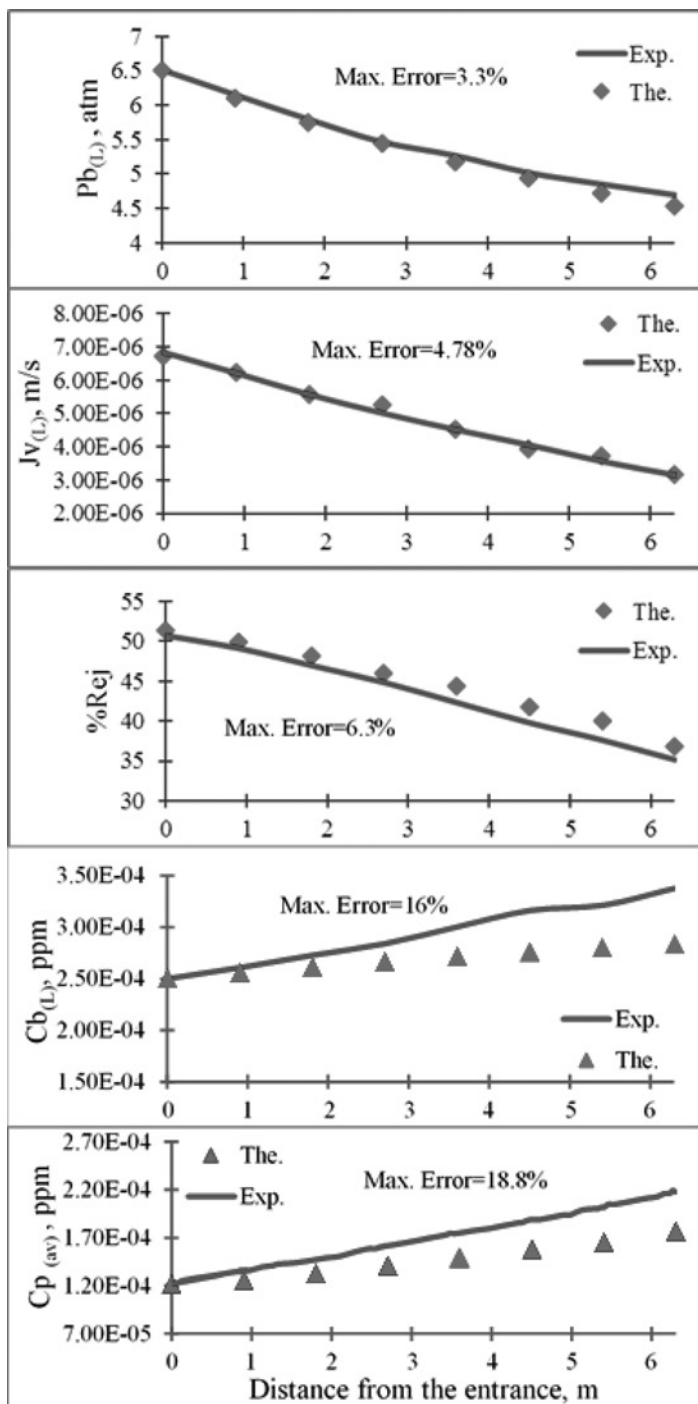


FIGURE 5.18 Experimental and model prediction of (a) retentate pressure, (b) outlet permeate flux, (c) NDMA rejection, (d) NDMA retentate concentration, and (e) NDMA average permeate concentration (feed conditions: 6.51 atm, 250E-6 ppm, 2.43E-3 m³/s and 20 °C).

(Adapted from Al-Obaidi et al., 2017g)

elements in a series configuration. However, the model was overestimating the retentate concentrations and the permeate concentration at the last membrane by around 16% and 18.8%, respectively. Seemingly, the model developed by Al-Obaidi et al. (2017c) has ignored the effect of fouling, where the water permeability constant has not included the propensity of fouling. Therefore, it is fair to expect a limited accuracy of model prediction of some parameters. Nevertheless, the model could predict the total NDMA rejection within a maximum error of 6.3%.

5.6.10 MODEL X: AL-OBDAIDI ET AL. (2017D)

Al-Obaidi et al. (2017d) developed a simple steady state lumped parameter model that can be used to simulate the phenomenon of solvent and solute transport through the membrane. This model incorporates the fluid physical properties to predict the rejection of organic compounds for a spiral wound RO process and multi-stage RO process. The development of this model was based on the same assumption used by the model of Al-Obaidi and Mujtaba (2016). However, the assumptions of constant solvent and solute transport parameters were relaxed by considering the impact of operating temperature on the membrane transport parameters.

5.6.10.1 Assumptions

The model assumes the following:

- A flat membrane sheet with negligible channel curvature.
- Validity of Darcy's law for the feed channel where the friction parameter is applied to express the pressure drop along the feed channel.
- The film model theory is used to estimate the concentration polarisation impact.
- Constant 1 atm pressure at the permeate side.
- The impact of operating temperature on the membrane transport parameters is considered.
- Negligible impact of feed spacer on the fluid patterns at the feed channel.
- Constant friction factor of feed channel is assumed due to laminar flow.

5.6.10.2 Model Equations

Key model equations are the following:

Water and solute fluxes through the membrane are represented as:

$$J_w = \frac{Q_p}{A} = A_w \left[\left(\frac{P_{f(in)} + P_{f(out)}}{2} - P_p \right) - \left(R(T + 273.15)(C_w - C_p) \right) \right] \quad (5.159)$$

$$J_s = B_{s(T_b)} (C_w - C_p) \quad (5.160)$$

The bulk concentration is calculated as the average value of feed and retentate concentrations:

$$C_b = \frac{C_f + C_r}{2} \quad (5.161)$$

The bulk feed velocity is calculated as:

$$U_b = \frac{Q_b}{W t_f \epsilon} \quad (5.162)$$

ϵ (dimensionless) is the void fraction of the spacer. The bulk feed flow rate is:

$$Q_b = \frac{Q_f + Q_r}{2} \quad (5.163)$$

Q_f and Q_r (m^3/s) are the feed and retentate flow rates. The process of organic compound rejection is followed by a pressure drop along the membrane edges. Therefore, the retentate pressure is calculated using the correlation of Al-Obaidi et al. (2017c).

$$P_{b(out)} = \left\{ P_{b(in)} - (b L Q_f) + \left(b W \theta \left(\frac{L^2}{2} \right) \Delta P_{b(out)} \right) - \left[b^2 W \theta \left(\frac{L^3}{6} \right) Q_f \right] - \left[b^2 W \theta \left(\frac{W \theta}{b} \right)^{0.5} \left(\frac{L^3}{6} \right) (\Delta P_{b(out)} - \Delta P_{b(in)}) \right] \right\} \quad (5.164)$$

θ is a dimensionless term defined as:

$$\theta = \frac{A_w B_s}{B_s + R (T + 273.15) A_w C_p} \quad (5.165)$$

The driving pressure is calculated as:

$$\Delta P_b = P_{b(in)} - \frac{P_{b(lose)}}{2} - P_p \quad (5.166)$$

The overall solute and mass balance equations are:

$$Q_f = Q_r + Q_p \quad (5.167)$$

$$Q_f C_f = Q_r C_r + Q_p C_p \quad (5.168)$$

Q_p (m^3/s) is the total permeate flow rate. The concentration at the permeate channel is:

$$C_p = \frac{C_f B_s(T_b)}{B_s(T_b) + \frac{J_w}{\exp\left(\frac{J_w}{k}\right)}} \quad (5.169)$$

The membrane rejection and water recovery are:

$$Rej = \frac{C_f - C_p}{C_f} \times 100 \quad (5.170)$$

$$Rec = \frac{Q_p}{Q_f} \times 100 \quad (5.171)$$

$$Q_p = J_w A \quad (5.172)$$

A (m²) is the effective membrane area.

The total energy consumption EI (kWh/m³) of RO system, measured in kWh per m³ of the total permeate, is calculated based on the use of a high-pressure pump (Qi et al., 2012).

$$EI = \frac{\left(\left(P_{b(0)} 101325 \right) F_{b(0)} \right)}{F_{p(Total)} \varepsilon_{pump}} \quad (5.173)$$

ε_{pump} (dimensionless) is the pump efficiency. The impact of operating temperature on water and solute transport parameters is shown in the equations of Sarkar et al. (2008) as follows:

$$A_{w(T+273.15)} = A_{w(T_{ref}+273.15)} \frac{\mu_{b(T_{ref}+273.15)}}{\mu_{b(T+273.15)}} \quad (5.174)$$

$$B_{s(T_b+273.15)} = B_{s(T_{ref}+273.15)} \frac{T_b + 273.15}{T_{ref} + 273.15} \frac{\mu_{b(T_{ref}+273.15)}}{\mu_{b(T_b+273.15)}} \quad (5.175)$$

T_{ref} (°C) is the reference temperature.

5.6.10.3 Model Validation

The water and solute transport parameters and the friction parameter of the model by Al-Obaidi et al. (2017d) were taken from the experimental work of Srinivasan et al. (2011) and Sundaramoorthy et al. (2011b) for the removal of dimethylphenol and chlorophenol, respectively, from wastewater. Figure 5.19 and Table 5.18 compare the experimental results of Srinivasan et al. (2011) and Sundaramoorthy et al. (2011b) against the model prediction of several operating parameters for the removal of dimethylphenol and chlorophenol from wastewater. The validation results show a good match between the model prediction and the experimental data as indicated by the high regression coefficient (R²) presented in Figure 5.19.

5.6.11 MODEL XI: AL-OBAIDI ET AL. (2018A)

The model of Al-Obaidi et al. (2018a) is in fact an upgrade of that of the Al-Obaidi et al. (2017d) model. This was carried out by a suitable moderation to predict

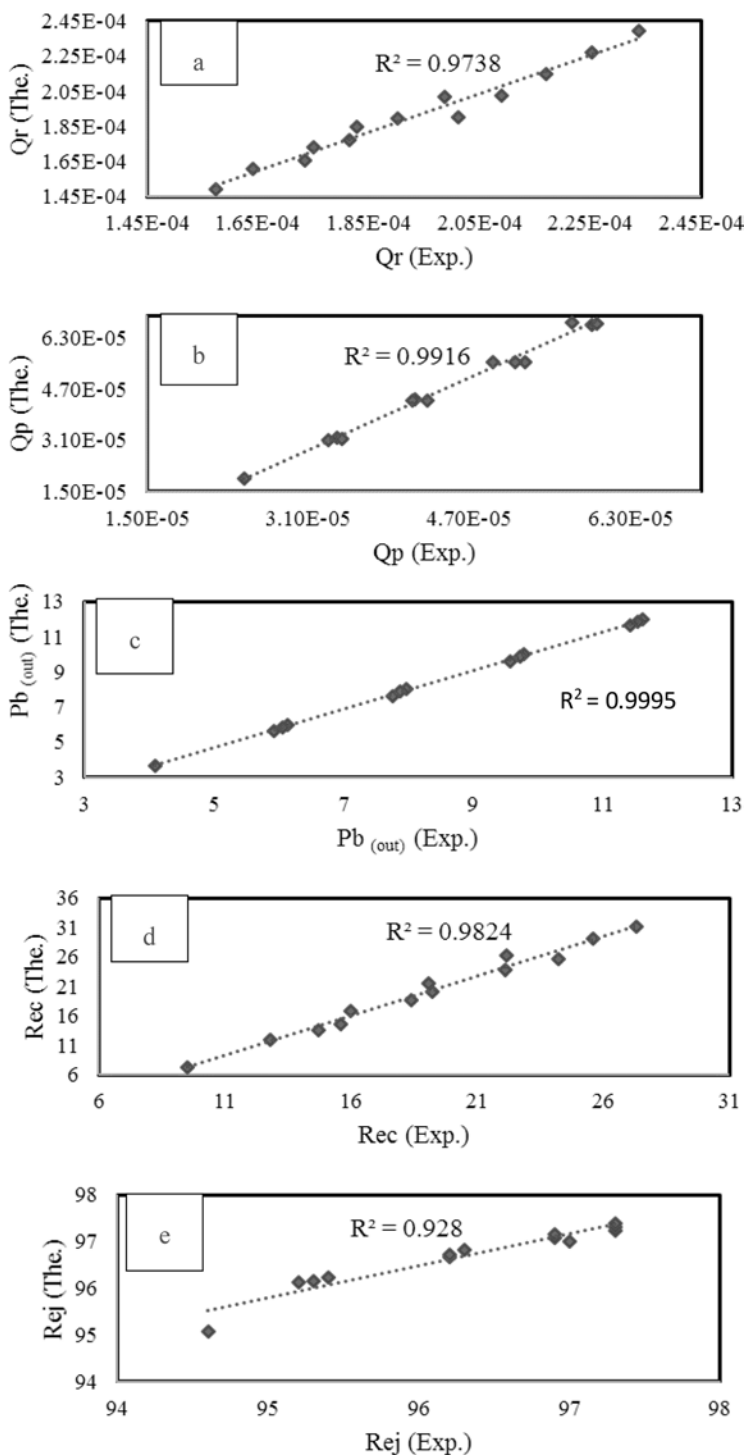


FIGURE 5.19 Comparison of model and experimental values of Srinivasan et al. (2011) (a: retentate flow rate, b: permeate flow rate, c: retentate pressure, d: total permeate recovery, and e: dimethylphenol rejection).

(Adapted with permission from Al-Obaidi et al., 2018e)

TABLE 5.18
Model Validation Results against Chlorophenol Removal of Sundaramoorthy et al. (2011b)

No	P _{b(in)} (atm)	C _p ×10 ³ (kmol/ m ³)	T (°C)	Q _f ×10 ⁴ (m ³ /s)	P _{b(out)} (atm) Exp. The.	%Error	Q _p ×10 ⁴ (m ³ /s) Exp. The.	%Error	C _p ×10 ³ (kmol/m ³) Exp. The.	%Error	Rej (-) Exp. The.	%Error	
1	9.71	0.778	30	2.166	8.3	8.16	1.6	1.59	1.63	-2.2	61.4	62.48	-1.7
2	11.64	0.778	30	2.166	10.08	10.14	-0.6	1.50	1.50	0.3	63.8	62.45	2.1
3	13.58	0.778	30	2.166	12.04	12.14	-0.8	1.37	1.37	0.3	66.2	62.21	6.0
4	7.77	6.226	31	2.166	6.24	6.145	1.5	1.82	1.84	-0.8	76.7	80.87	-5.4
5	9.71	6.226	31	2.166	8.11	8.129	-0.2	1.75	1.73	0.9	79.8	82.54	-3.4
6	11.64	6.226	31	2.166	9.98	10.10	-1.2	1.64	1.62	0.9	81	83.62	-3.2
7	13.58	6.226	31	2.166	11.85	12.08	-1.9	1.57	1.52	3.5	81.9	84.38	-3.0
8	5.83	0.778	30	2.33	4.46	4.04	9.3	1.95	2.06	-5.2	56.2	61.59	-9.5
9	7.77	0.778	30	2.33	6.35	6.03	4.9	1.86	1.93	-3.5	58.1	62.86	-8.2
10	9.71	0.778	30	2.33	8.22	8.03	2.2	1.74	1.79	-2.8	60.3	63.26	-4.9
11	11.64	0.778	30	2.33	10.09	10.01	0.7	1.63	1.66	-1.3	62.4	63.26	-1.3
12	13.58	0.778	30	2.33	11.96	12.00	-0.3	1.54	1.53	0.7	64.5	63.05	2.2
13	5.83	6.226	31	2.33	4.27	4.02	5.6	2.08	2.12	-1.9	74.5	78.15	-4.9
14	7.77	2.455	31	2.33	6.16	6.01	2.4	1.98	2.01	-1.1	76.6	81.15	-5.9
15	9.71	2.455	31	2.33	8.03	7.99	0.4	1.90	1.90	0.2	79.8	82.83	-3.8
16	11.64	2.455	31	2.33	9.9	9.97	-0.7	1.81	1.79	1.5	81.2	83.91	-3.3
17	13.58	2.455	31	2.33	11.77	11.95	-1.5	1.73	1.68	3.1	82.2	84.68	-3.0
18	7.77	1.556	31	2.583	6.17	5.82	5.5	2.14	2.20	-2.3	67.5	73.65	-9.1
19	9.71	1.556	31	2.583	7.79	7.81	-0.3	2.04	2.07	-1.3	69.7	74.83	-7.3
20	11.64	1.556	31	2.583	9.92	9.79	1.2	1.94	1.94	0.2	71.2	75.51	-6.0
21	13.58	1.556	31	2.583	11.79	11.79	-0.0	1.85	1.81	1.9	72.5	75.93	-4.7
22	9.71	2.335	31	2.583	8.03	7.81	2.7	2.08	2.09	-0.3	72.8	77.91	-7.0
23	11.64	2.335	31	2.583	9.84	9.79	0.4	1.97	1.96	0.3	74.2	78.75	-6.1
24	13.58	2.335	31	2.583	11.74	11.78	-0.3	1.86	1.84	1.4	75.7	79.30	-4.7
25	7.77	6.226	31	2.583	6.03	5.80	3.7	2.25	2.26	-0.5	77.8	81.52	-4.7
26	9.71	6.226	31	2.583	7.9	7.79	1.3	2.17	2.15	0.8	79.4	83.23	-4.8
27	11.64	6.226	31	2.583	9.75	9.76	-0.1	2.09	2.04	2.4	81.5	84.33	-3.4
28	13.58	6.226	31	2.583	11.65	11.74	-0.8	2.01	1.93	4.1	83	85.10	-2.5

(Adapted from Al-Obaidi et al., 2018f)

accurately the performance of a spiral wound RO process for the rejection of high-toxic N-nitrosamine compounds from wastewater. For this to happen, the interaction between transport theories through the membrane needed to be represented mathematically for building an appropriate numerical model, which would incorporate the calculations of the fluid properties. For this purpose, a new assumption was considered for the new proposed model as follows:

- Validity of the Da Costa equation to predict the pressure drop across the membrane.

The model was developed for N-nitrosamine compounds. Therefore, a set of new equations was considered as described below.

The feed and permeate osmotic pressure are obtained based on the proposed correlations of Fujioka et al. (2014).

$$\pi_m = 1.19(T_b + 273.15) \left(\frac{C_w}{M_{wt}} \right) \quad (5.176)$$

$$\pi_p = 1.19(T_b + 273.15) \left(\frac{C_p}{M_{wt}} \right) \quad (5.177)$$

M_{wt} (kg/kmol) is the molecular weight of the selected compound of N-nitrosamine.

The process of NDMA rejection is accompanied by a pressure drop along the membrane edges. Therefore, the retentate pressure is calculated as:

$$P_{f(out)} = P_{f(in)} - \Delta P_{drop} \quad (5.178)$$

The pressure drop of the spiral wound element has been calculated from the proposed correlation of Da Costa et al. (1994) in line with the previously mentioned assumption. Da Costa et al. (1994) assumes that the pressure losses and kinetic losses are happening due to drag on the feed spacer and a change in direction of flow, respectively, and neglecting the friction losses at the channel walls and on the spacer surface.

$$\Delta P_{drop} = \left(\frac{\rho_b U_b^2 L C_{td}}{2 d_h} \right) \times 9.8692 \times 10^{-6} \quad (5.179)$$

C_{td} and d_h (dimensionless, m) are the total drag coefficient and hydraulic diameter of the feed spacer channel, respectively.

$$C_{td} = \frac{A'}{Re^n} \quad (5.180)$$

A' and n (dimensionless) are the spacer characteristics.

The Reynolds number is calculated as:

$$Re = \frac{\rho_b d_h U_b}{\mu_b} \quad (5.181)$$

d_h (m) is the hydraulic diameter.

The total energy consumption of the RO system measured in kWh per m³ for the use of high-pressure (E1) is calculated using Eq. (5.173). However, in the case of using an energy recovery device (ERD) in the RO process network, the total energy consumption E2 (kWh/m³) has considered both the high pressure and ERD. More specifically, the energy performance of the conventional pilot plant is calculated regarding the outgoing and ingoing entering energies.

$$E2 = \frac{\frac{(P_{b(0)} 101325) F_{b(0)}}{F_{p(Total)}} \varepsilon_{pump} - \frac{(P_{b(L)} 101325) F_{b(L)} \varepsilon_{ERD}}{F_{p(Total)}}}{36E5}$$

(5.182)

Eq. (5.183) calculates the outlet pressure of the ERD, which is used in the next stage, i.e. the outlet pressure of the membrane modules of the previous stage $P_{f(in)(ERD)}$.

$$\varepsilon_{ERD} = \frac{P_{b(ERD)}}{P_{b(L)}}$$

(5.183)

5.6.11.1 Parameters Estimation

The parameter estimation method using the gPROMS software, as described earlier, was used to predict the accurate values of the water permeability constant, the NDMA transport parameter, and the spacer characteristics of A' and n, based on the same experimental data of NDMA removal from wastewater of Fujioka et al. (2014). Table 5.19 shows the model parameters. The estimated dimensions of the spacer mesh (A' and n) were found to be close to the spacer type CONWED-1 as reported in the study of Da Costa et al. (1994) (A' = 1.29 and n = 0.24).

5.6.11.2 Model Validation

The predictions of the model by Al-Obaidi et al. (2018a) were compared with the experimentation data of Fujioka et al. (2014) for three elements of spiral wound RO process in a series configuration. Table 5.20 compares the values of retentate plant flow rate, total permeate flux, and total NDMA rejection. The results clearly show that the predicted values using the model are consistent with the experimental ones.

TABLE 5.19
Parameter Estimation Results

Parameter	Value
$A_{w(T)}$	1.1290×10^{-6} (m/s atm)
$B_{s(T)}$	4.0919×10^{-6} (m/s)
A' (–)	1.47
n (–)	0.24

(Adapted from Al-Obaidi et al., 2018a)

TABLE 5.20
Model Validation Results

$P_{f(in)}$ (atm)	$J_w(m/s) \times 10^6$		Error %	$Q_f(m^3/s) \times 10^3$		Error %	Rej (–)		Error %
	Exp.	Model		Exp.	Model		Exp.	Model	
4	2.78	2.73	1.67	2.36	2.37	–0.22	0.38	0.39	–0.60
6.51	5.56	5.58	–0.41	2.30	2.29	0.100	0.56	0.55	0.96

$C_{f(NDMA)} = 250 \text{ ng / L}$, $Q_f = 2.43 \times 10^{-3} \text{ m}^3/\text{s}$, and $T = 20 \text{ }^\circ\text{C}$

(Adapted from Al-Obaidi et al., 2018a)

5.6.12 MODEL XII: AL-OBaidi ET AL. (2018B)

Several organic and non-organic compounds are found in the wastewater of several industries. The models reviewed so far are suitable for the application of a spiral wound RO process for the removal of a single organic pollutant from wastewater. The available literature includes a few more models that can be used for predicting the removal of multi-components from wastewater. However, these models were developed as lumped parameter models, which ignored the spatial variation of operating parameters along the axes of the membrane. For instance, a lumped parameter model was developed by Al-Bastaki (2004) to investigate the performance of a spiral wound RO process for the removal of Na₂SO₄ and methyl orange dye from wastewater. In contrast with such attempts, Al-Obaidi et al. (2018b) developed a distributed one-dimensional model for predicting the transport phenomena of a multi-compounds RO process for wastewater treatment.

5.6.12.1 Assumptions

The following new assumptions were considered to build this model.

- A flat membrane sheet with negligible channel curvature.
- The variation of operating conditions along y-axis is ignored.
- Validity of Darcy’s law for the feed channel where the friction parameter is applied to characterise the pressure drop.
- The contribution of all the compounds to the osmotic pressure is considered.
- Validity of the film model theory to estimate the concentration polarisation impact.
- Constant 1 atm pressure at the permeate side.
- A constant solute concentration is assumed in the permeate channel and the average value will be calculated from the inlet and outlet permeate solute concentrations.
- The underlying process is isothermal. Therefore, the temperatures of the feed, retentate, and permeate are equal.
- Negligible impact of feed spacer on the fluid patterns at the feed channel.
- Constant membrane transport parameters.
- Constant friction factor of feed channel is assumed due to laminar flow.

5.6.12.2 Model Equations

Key equations developed in this model are shown in this section.

Permeate flux at any point along the x-axis is calculated as:

$$J_{v(x)} = A_w \left\{ \Delta P_{b(x)} - \left[\sum_i^n (R(T_b + 273.15) \left(\frac{J_{v(x)} C_{p(i)(x)}}{B_{s(i)}} \right)) \right] \right\} \quad (5.184)$$

The second term of the above equation represents the total osmotic pressure.

The solute flux of each component is:

$$J_{s(i)(x)} = B_{s(i)} (C_{w(i)(x)} - C_{p(i)(av)}) \quad (5.185)$$

i and n are the solute under consideration and the total number of solutes, respectively.

Operating pressure along the feed channel is given as:

$$\Delta P_{b(x)} = P_{b(x)} - P_p \quad (5.186)$$

Bulk solute concentration is estimated as:

$$\begin{aligned} \frac{C_{b(i)(x)}}{t_f W} \frac{dF_{b(x)}}{dx} + \frac{F_{b(x)}}{t_f W} \frac{dC_{b(i)(x)}}{dx} = \frac{d}{dx} \left[D_{b(i)(x)} \frac{dC_{b(i)(x)}}{dx} \right] \\ - \frac{(J_{w(x)} C_{p(i)(x)})}{t_f} + \frac{(J_{w(x)} C_{b(i)(x)})}{t_f} \end{aligned} \quad (5.187)$$

The last term of Eq. (5.187) represents the change of bulk concentration due to solvent through the membrane. Permeate solute concentration of each solute at $x = 0$ and $x = L$ are calculated as:

$$C_{p(i)(0)} = \frac{B_{s(i)} C_{b(i)(0)} e^{\frac{J_{w(0)}}{k(i)(0)}}}{J_{w(0)} + B_{s(i)} e^{\frac{J_{w(0)}}{k(i)(0)}}} \quad C_{p(i)(L)} = \frac{B_{s(i)} C_{b(i)(L)} e^{\frac{J_{w(L)}}{k(i)(L)}}}{J_{w(L)} + B_{s(i)} e^{\frac{J_{w(L)}}{k(i)(L)}}} \quad (5.188)$$

However, the average permeate concentration of each solute is estimated as:

$$C_{p(i)(av)} = \frac{C_{p(i)(0)} + C_{p(i)(L)}}{2} \quad (5.189)$$

Wall solute concentration of each solute is given as:

$$\frac{(C_{w(i)(x)} - C_{p(i)(av)})}{(C_{b(i)(x)} - C_{p(i)(av)})} = \exp \left(\frac{J_{w(x)}}{k(i)(x)} \right) \quad (5.190)$$

5.6.12.3 Model Validation

The model developed by Al-Obaidi et al. (2018b) was validated against the experimental data of Sundaramoorthy et al. (2011b) for the removal of a single compound (chlorophenol) from wastewater due to the absence of experimental data in the literature for the removal of multi-compounds from wastewater.

Therefore, the water permeability constant and friction factor are taken from Sundaramoorthy et al. (2011b) and the solute transport parameters of the selected compounds were gathered from the literature and are given in Table 5.21. The model showed good agreement between solute rejection and water recovery as presented in Figure 5.20.

The next sections describe in detail the model developed by Al-Obaidi et al. (2017e), which is based on the irreversible thermodynamic model.

TABLE 5.21
Physical and Transport Parameters of the Eight Selected Organic Compounds

Contaminant	Membrane	B_s (m/s)	Source
Dimethylphenol	Ion Exchange, India	1.5876×10^{-8}	(Srinivasan et al., 2011)
Chlorophenol	Ion Exchange, India	8.4680×10^{-8}	(Sundaramoorthy et al., 2011b)
Phenol	Permionics, India	6.5367×10^{-7}	(Srinivasan et al., 2010)
Methyl orange dye	FilmTec SW30	3.2000×10^{-9}	(Al-Bastaki, 2004)
Aniline	DESAL-3B	4.1900×10^{-6}	(Hidalgo et al., 2014)
Ammonium	SEPA-SSIC	1.1696×10^{-7}	(Bódalo et al., 2005)
Cyanide	DESAL-3	2.1861×10^{-6}	(Bódalo et al., 2004)
Sulphate	SEPA-SSIC	3.9869×10^{-8}	(Bódalo et al., 2003)

(Adapted from Al-Obaidi et al., 2018b)

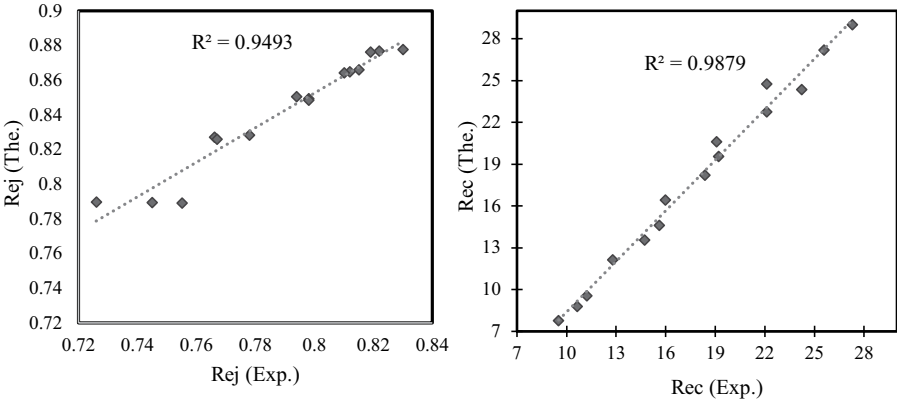


FIGURE 5.20 Model validation results.

(Adapted from Al-Obaidi et al., 2018b)

5.6.13 MODEL XIII: AL-OBAYDI ET AL. (2017E)

A new explicit one-dimensional steady state model based on the three-parameter Spiegler-Kedem methodology (irreversible thermodynamic model) was developed to predict the performance of a spiral wound RO process for the rejection of organic compounds from wastewater.

5.6.13.1 Assumptions

- A flat membrane sheet with negligible channel curvature.
- Validity of Darcy's law for the feed channel where the friction parameter is applied to characterise the pressure drop.
- Validity of the film model theory to estimate the concentration polarisation impact.
- Constant 1 atm pressure at the permeate side.
- A constant solute concentration is assumed in the permeate channel and the average value will be calculated from the inlet and outlet permeate solute concentrations.
- The underlying process is isothermal.
- Negligible impact of feed spacer on the fluid patterns at the feed channel.
- Constant friction factor of feed channel is assumed due to laminar flow.

5.6.13.2 Model Equations

The volumetric water and molar solute fluxes at each point along the x-axis are:

$$J_{w(x)} = \frac{L_p (\Delta P_{b(x)})}{1 + \frac{\sigma C_{p(av)} L_p}{\omega} - \frac{C_{b(av)}^* (1 - \sigma) L_{p\sigma}}{\omega}} \quad (5.191)$$

$$J_{s(x)} = J_{w(x)} (1 - \sigma) C_{b(av)}^* + \omega RT_b (C_{w(x)} - C_{p(av)}) \quad (5.192)$$

The average bulk concentration is expressed as the average values of inlet and retentate concentrations as follows:

$$C_{b(av)}^* = \frac{C_{b(0)}^* + C_{b(L)}^*}{2} \quad (5.193)$$

$$C_{b(0)}^* = \frac{C_{b(0)} - C_{p(av)}}{\ln \left(\frac{C_{b(0)}}{C_{p(av)}} \right)} \quad \text{and} \quad C_{b(L)}^* = \frac{C_{b(L)} - C_{p(av)}}{\ln \left(\frac{C_{b(L)}}{C_{p(av)}} \right)} \quad (5.194)$$

The osmotic pressure at each point along the x-axis is:

$$\Delta\pi_{(x)} = \frac{J_{w(x)}C_{p(av)}}{\omega} - \frac{J_{w(x)}(1-\sigma)C_{b(av)}}{\omega} \quad (5.195)$$

Feed flow rate and feed pressure at any point along x-axis of the feed channel are:

$$F_{b(x)} = \frac{F_{b(L)} \left(e^{\sqrt{\frac{L_p}{Z}} x} - e^{-\sqrt{\frac{L_p}{Z}} x} \right) + F_{b(0)} \left(e^{\sqrt{\frac{L_p}{Z}} (L-x)} - e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right)}{\left(e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \quad (5.196)$$

$$P_{b(x)} = P_{b(0)} - \frac{b}{\sqrt{\frac{L_p}{Z}} \left(e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \left\{ \left[F_{b(L)} \left[e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} - 2 \right] \right. \right. \\ \left. \left. - F_{b(0)} \left[\left(e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) - \left(e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right) \right] \right] \right\} \quad (5.197)$$

$$Z = \frac{1 + \frac{\sigma C_{p(av)} L_p}{\omega} - \frac{C_{b(av)} (1-\sigma) L_{p\sigma}}{\omega}}{W b} \quad (5.198)$$

The pressure difference between the feed and permeate channel along the x-axis is written as:

$$\Delta P_{b(x)} = \frac{\sqrt{\frac{L_p}{Z}} Z b \left\{ \left[F_{b(0)} \left(e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) \right] - \left[F_{b(L)} \left(e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} \right) \right] \right\}}{L_p \left(e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \quad (5.199)$$

The retentate flow rate at $x = L$ is:

$$F_{b(L)} = \frac{F_{b(0)} \left(e^{\sqrt{\frac{L_p}{Z}} L} + e^{-\sqrt{\frac{L_p}{Z}} L} \right)}{2} - \frac{\Delta P_{b(0)} \sqrt{\frac{L_p}{Z}} \left(e^{\sqrt{\frac{L_p}{Z}} L} + e^{-\sqrt{\frac{L_p}{Z}} L} \right)}{2b} \quad (5.200)$$

Then, another equation for water flux was derived as:

$$J_{w(x)} = \frac{\sqrt{\frac{L_p}{Z}}}{W \left(e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \left\{ \left[F_{b(0)} \left(e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) \right] - \left[F_{b(L)} \left(e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} \right) \right] \right\} \quad (5.201)$$

Bulk solute concentration (Chen-Jen et al., 2010) and permeate concentration at any point along the x-axis of feed and permeate channels are:

$$\frac{d \left(\frac{C_{b(x)} F_{b(x)}}{t_f W} \right)}{dx} = - \frac{J_{w(x)} C_{p(av)}}{t_f} + \frac{J_{w(x)} C_{b(x)}}{t_f} + \frac{d}{dx} \left(D_{b(x)} \frac{dC_{b(x)}}{dx} \right) \quad (5.202)$$

$$C_{p(av)} = \frac{C_{b(av)}^{\sim} (1-\sigma) J_{w(x)} + \omega R T_b C_{b(x)} e^{\frac{J_{w(x)}}{k(x)}}}{J_{w(x)} + \omega R T_b e^{\frac{J_{w(x)}}{k(x)}}} \quad (5.203)$$

To simplify Eq. (5.203), the reflection coefficient will be assumed as ($\sigma = 1$), then:

$$C_{p(av)} = \frac{\omega R T_b C_{b(x)} e^{\frac{J_{w(x)}}{k(x)}}}{J_{w(x)} + \omega R T_b e^{\frac{J_{w(x)}}{k(x)}}} \quad (5.204)$$

Eq. (5.204) can be rewritten in the form of Eq. (5.205) to be compatible with calculating the average permeate solute concentration by considering the solution-diffusion model.

$$C_{p(av)} = \frac{B_s C_{b(x)} e^{\frac{J_{w(x)}}{k(x)}}}{J_{w(x)} + B_s e^{\frac{J_{w(x)}}{k(x)}}} \quad (5.205)$$

Eq. (5.205) is used in both ($x = 0$ and $x = L$) and then the average value is taken as the average solute concentration in the permeate channel.

The model was also used to predict the removal of phenol from wastewater based on the experiments of Srinivasan et al. (2010). Therefore, a new equation for the mass transfer coefficient of phenol was investigated according to experimental data to show the impact of solvent flux, flow rate, solute concentration, and both the solvent and solute properties. The impact of all these factors can be correlated in Eq. (5.163) as follows:

$$Sh_{(x)} = c_1 \left[Re_{p(x)} Re_{f(x)} C_{m(x)} Sc_{p(x)} Sc_{f(x)} \right]^{c_2} \quad (5.206)$$

$$Sh = \frac{2 t_f k_{(x)}}{D_{b(x)}} \quad Sc_{p(x)} = \frac{\mu_{p(x)}}{\rho_{p(x)} D_{p(x)}} \quad Sc_{b(x)} = \frac{\mu_{b(x)}}{\rho_{b(x)} D_{b(x)}} \quad (5.207)$$

$Sh_{(x)}$, $Sc_{p(x)}$, $Sc_{f(x)}$ are the Sherwood number, the permeate Schmidt number, and the feed Schmidt number at any point along the x-axis, respectively. In order to speculate the values of (c_1 and c_2) mentioned in Eq. (5.206), the mass transfer coefficients will be calculated from the correlation reported by Wankat (1990):

$$k_{(x)} = 1.177 \left(\frac{F_{b(x)} D_{b(x)}^2}{t_f^2 W L} \right)^{0.333} \quad (5.208)$$

Then, the other parameters of Eq. (5.206) in both ($x = 0$ and $x = L$) can be estimated from the experimental data of phenol, which were reported by Srinivasan et al. (2010).

Finally, by plotting $\ln(Sh)$ against $\ln(Re_p Re_b C_m Sc_p Sc_b)$, the constants can be found. As a result, the mass transfer coefficient of phenol is given by:

$$k_{(x)} = \frac{6.5045 D_{b(x)}^{0.9995}}{t_f} \left(\frac{F_{b(x)} t_p J_{w(x)} C_{s(x)}}{W \rho_m D_{p(x)}} \right)^{0.0005} \quad (5.209)$$

Note: an extended version of this model is presented in Chapter 9 (Model XV).

5.6.13.3 Parameters Estimation

The parameter estimation tool gEST in the gPROMS (described earlier) was used in the model by Al-Obaidi et al. (2017e) for predicting the unknown parameters L_p , ω , B_s , σ , and b of the model. These were based on the experimental work of Srinivasan et al. (2010). The parameter estimation results reported in Table 5.22 show the variation of transport parameters with the inlet feed solute concentration for the experimental work.

5.6.13.4 Model Validation

Table 5.23 shows the experimental results of phenol removal and the model predictions for five groups of inlet feed solute concentration (each group holding six

TABLE 5.22
Results of Parameter Estimation

$C_{b(0)} \times 10^3 (\text{kmol/m}^3)$	T_b (°C)	$P_{b(0)} (\text{atm})$	$L_p \times 10^6$ (m/atm s)	$\omega \times 10^6 (\text{kmol/m}^2 \text{ s atm})$	$B_s \times 10^6 (\text{m/s})$
2.125	32.5	4.93	1.404	5.238	1.734
2.125	33.1	6.9	1.404	5.238	1.734
2.125	33.0	8.9	1.404	5.238	1.734
2.125	33.2	10.9	1.404	5.238	1.734
2.125	34.0	14.8	1.404	5.238	1.734
4.25	32.2	4.93	1.248	0.677	1.070
4.25	32.8	6.9	1.248	0.677	1.070
4.25	33.5	8.9	1.248	0.677	1.070
4.25	33.9	10.9	1.248	0.677	1.070
4.25	34.5	12.8	1.248	0.677	1.070
4.25	34.5	14.8	1.248	0.677	1.070
6.375	32.5	4.93	1.131	1.521	0.841
6.375	33.0	6.9	1.131	1.521	0.841
6.375	33.2	8.9	1.131	1.521	0.841
6.375	33.5	10.9	1.131	1.521	0.841
6.375	33.8	12.8	1.131	1.521	0.841
6.375	34.0	14.8	1.131	1.521	0.841
8.5	32.0	4.93	1.209	1.858	1.147
8.5	32.5	6.9	1.209	1.858	1.147
8.5	32.8	8.9	1.209	1.858	1.147
8.5	33.0	10.9	1.209	1.858	1.147
8.5	33.2	12.8	1.209	1.858	1.147
8.5	33.5	14.8	1.209	1.858	1.147
10.6	31.5	4.93	1.118	0.5885	1.097
10.6	32.2	6.9	1.118	0.5885	1.097
10.6	32.6	8.9	1.118	0.5885	1.097
10.6	32.8	10.9	1.118	0.5885	1.097
10.6	32.8	12.8	1.118	0.5885	1.097
10.6	33.0	14.8	1.118	0.5885	1.097
$b = 13,000 \text{ atm s/m}^4$			$\sigma = 0.9075$		

(Adapted from Al-Obaidi et al., 2018b)

different inlet feed pressures). Table 5.23 also shows the percentage error between the experimental results and the model predictions for several model parameters. Figure 5.21 shows the comparison of experimental and theoretical results for an average solute rejection and an average permeate concentration. Generally, the predicted values of the theoretical model are in a good agreement with the experimental ones over the ranges of pressure and concentration.

TABLE 5.23
Validation with Experimental Results of Phenol for the Feed Flow Rate ($F_{b(0)} = 3.333 \times 10^{-4} \text{ m}^3/\text{s}$)

No	$P_{b(0)}$ atm	$C_{b(0)} \times 10^3$ (kmol/m ³)	T_b °C	$P_{b(t)}$ (atm)		$C_{p(a0)} \times 10^3$ (kmol/m ³)		%Error		$F_{p(\text{total})} \times 10^6$ (m ³ /s)		%Error		$\text{Re}_{j(\text{av})}$		%Error		$\text{Fb(L)} \times 10^4$ (m ³ /s)		%Error
				Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	Exp.	The.	
1	4.93	2.125	32.5	2.99	2.99	0.01	0.831	0.80	3.02	3.53	3.02	14.4	0.646	0.63	0.646	0.63	-3.14	3.30	3.30	-0.12
2	6.9	2.125	33.1	4.96	4.97	0.13	0.647	0.63	1.54	5.20	5.18	0.45	0.727	0.71	0.727	0.71	-2.66	3.28	3.28	-0.00
3	8.9	2.125	33	6.9	6.97	1.04	0.580	0.57	0.96	7.20	7.37	-2.30	0.759	0.74	0.759	0.74	-2.62	3.26	3.26	0.03
4	10.9	2.125	33.2	8.9	8.98	0.87	0.524	0.55	-5.17	9.60	9.55	0.48	0.786	0.75	0.786	0.75	-4.35	3.24	3.24	-0.06
5	14.8	2.125	34	12.9	12.88	0.15	0.349	0.36	-5.55	12.2	12.2	0.00	0.874	0.83	0.874	0.83	-4.37	3.21	3.21	-0.07
6	4.93	4.25	32.2	2.99	2.99	0.00	1.24	1.24	-0.19	3.30	2.68	18.7	0.766	0.71	0.766	0.71	-7.61	3.30	3.31	-0.16
7	6.9	4.25	32.8	4.96	4.96	0.09	1.05	0.93	10.94	5.00	4.60	8.06	0.813	0.78	0.813	0.78	-3.54	3.28	3.29	-0.12
8	8.9	4.25	33.5	6.9	6.97	1.00	0.80	0.81	-1.22	7.00	6.54	6.54	0.861	0.81	0.861	0.81	-5.46	3.26	3.27	-0.16
9	10.9	4.25	33.9	8.9	8.98	0.84	0.72	0.75	-4.84	8.50	8.49	0.15	0.873	0.83	0.873	0.83	-5.21	3.25	3.25	-0.04
10	12.8	4.25	34.5	10.9	10.88	-0.17	0.685	0.73	-6.62	10.25	10.3	-0.82	0.880	0.84	0.880	0.84	-5.14	3.23	3.23	-0.03
11	14.8	4.25	34.5	12.9	12.89	0.0	0.718	0.73	-2.20	12.25	12.3	-0.23	0.876	0.84	0.876	0.84	-4.53	3.21	3.21	-0.07
12	4.93	6.375	32.5	2.99	2.99	0.00	1.40	1.65	-17.89	3.20	2.43	20.4	0.798	0.74	0.798	0.74	-7.22	3.30	3.31	-0.21
13	6.9	6.375	33	4.96	4.96	0.00	1.24	1.21	2.47	4.33	4.17	3.70	0.821	0.82	0.821	0.82	-0.86	3.29	3.29	-0.04
14	8.9	6.375	33.2	6.9	6.97	0.98	1.176	1.03	12.15	5.93	5.93	-0.06	0.834	0.84	0.834	0.84	1.02	3.27	3.27	-0.02
15	10.9	6.375	33.5	8.9	8.97	0.81	0.94	0.95	-1.05	7.00	7.70	-9.96	0.868	0.86	0.868	0.86	-1.25	3.26	3.26	0.17
16	12.8	6.375	33.8	10.9	10.9	0.00	0.87	0.91	-4.94	8.70	9.37	-7.73	0.879	0.86	0.879	0.86	-1.82	3.25	3.24	0.15
17	14.8	6.375	34	12.9	12.9	0.00	0.63	0.66	-6.12	11.1	11.1	0.00	0.914	0.90	0.914	0.90	-1.39	3.22	3.22	-0.07
18	4.93	8.50	32	2.99	2.99	0.00	2.61	2.65	-1.60	3.13	2.60	17.0	0.706	0.69	0.706	0.69	-2.00	3.30	3.31	-0.14
19	6.9	8.50	32.5	4.96	4.96	0.08	2.22	2.01	9.64	4.53	4.45	1.68	0.750	0.77	0.750	0.77	2.54	3.29	3.29	-0.02
20	8.9	8.50	32.8	6.9	6.97	0.99	1.93	1.75	9.58	6.20	6.34	-2.22	0.783	0.80	0.783	0.80	2.27	3.27	3.27	0.02
21	10.9	8.50	33	8.9	8.97	0.83	1.60	1.63	-1.94	8.20	8.22	-0.26	0.826	0.81	0.826	0.81	-1.18	3.25	3.25	-0.03
22	12.8	8.50	33.2	10.9	10.9	0.00	1.47	1.59	-8.16	9.30	10.0	-7.65	0.840	0.82	0.840	0.82	-2.11	3.24	3.23	0.16

23	14.8	8.50	33.5	12.9	12.9	0.00	1.40	1.59	-13.31	11.5	11.9	-3.43	0.849	0.82	-2.96	3.22	3.22	0.04
24	4.93	10.6	31.5	2.99	2.99	0.00	3.09	3.35	-8.40	2.66	2.40	9.94	0.711	0.68	-3.38	3.31	3.31	-0.06
25	6.9	10.6	32.2	4.96	4.96	0.00	2.52	2.51	0.39	4.13	4.11	0.47	0.764	0.76	0.47	3.29	3.29	-0.00
26	8.9	10.6	32.6	6.9	6.97	0.97	2.02	2.16	-6.92	5.86	5.85	0.14	0.816	0.80	-1.72	3.27	3.28	-0.02
27	10.9	10.6	32.8	8.9	8.97	0.81	1.83	2.00	-9.16	7.50	7.59	-1.24	0.835	0.81	-1.95	3.26	3.26	-0.01
28	12.8	10.6	32.8	10.9	10.9	0.00	1.69	1.94	-14.53	9.00	9.25	-2.73	0.846	0.82	-2.40	3.24	3.24	0.02
29	14.8	10.6	33	12.9	12.9	0.00	1.40	1.50	-7.10	10.5	10.5	-0.44	0.873	0.86	-0.84	3.23	3.23	-0.06

(Adapted from Al-Obaidi et al., 2018b)



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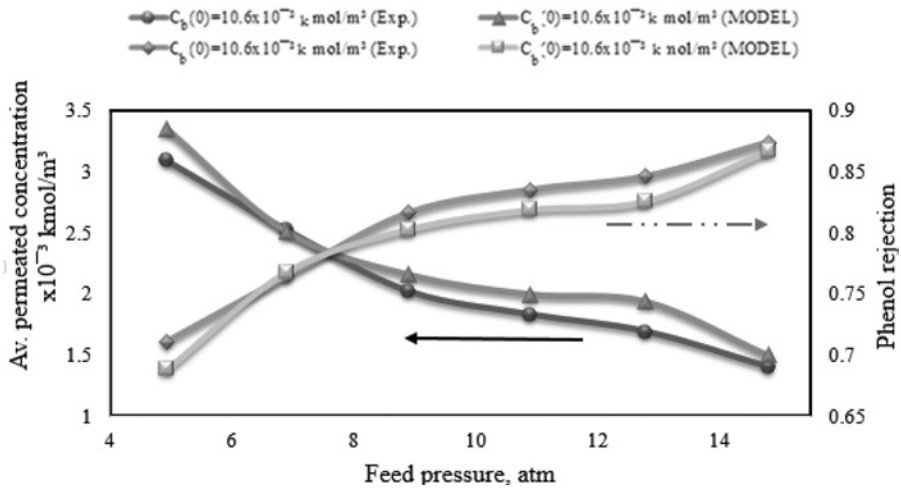


FIGURE 5.21 Comparison of theoretical and experimental results of phenol rejection and average permeate concentration.

(Adapted from Al-Obaidi et al., 2017e)

5.6.14 MODEL XIV: AL-OBaidi ET AL. (2017f)

A one-dimensional steady state model was developed by Al-Obaidi et al. (2017f) based on the validity of the Spiegler-Kedem model for the transport of water and solute through the membrane and complete mixing in the y-axis of the feed channel due to the existence of a network of spacers. The model investigated the performance of a spiral wound RO process for the removal of chemicals from wastewater but ignored the influence of fouling due to very low concentration of wastewater. The assumptions reported in the Al-Obaidi et al. (2017e) model were similarly used in the development of the model by Al-Obaidi et al. (2017f).

5.6.14.1 Model Equations

The new equations used in this model are given in this section.

The water flux and osmotic pressure at any point along the x-axis are:

$$J_{w(x)} = \frac{L_p}{\bar{\phi}_{(x)}} \left[\Delta P_{b(0)} - b x F_{b(0)} - b x \Delta P_{b(x)} \left(\frac{W L_p}{b \bar{\phi}_{(x)}} \right)^{0.5} + b x \Delta P_{b(0)} \left(\frac{W L_p}{b \bar{\phi}_{(x)}} \right)^{0.5} \right] \quad (5.210)$$

$$\bar{\phi}_{(x)} = 1 + \frac{\sigma C_{p(av)} L_p}{\omega} - \frac{C_{s(x)} (1 - \sigma) \sigma L_p}{\omega} \quad (5.211)$$

$$\Delta\pi_{s(x)} = \frac{J_{w(x)} C_{p(av)}}{\omega} - \frac{J_{w(x)} (1-\sigma) C_{s(x)}}{\omega} \quad (5.212)$$

The feed pressure, pressure difference between the feed and permeate channels, and feed flow rate at any point along the membrane length are:

$$\begin{aligned} P_{b(x)} &= P_{b(0)} - \left[b F_{b(0)} x \right] \\ &+ \left[b \left(\frac{W L_p}{\varnothing_{(x)}} \right) \left(\frac{x^2}{2} \right) \Delta P_{b(0)} \right] - \left[b^2 \left(\frac{W L_p}{\varnothing_{(x)}} \right) F_{b(0)} \left(\frac{x^3}{6} \right) \right] \\ &- \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{1.5} \Delta P_{b(x)} \left(\frac{x^3}{6} \right) \right] \\ &+ \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{1.5} \Delta P_{b(0)} \left(\frac{x^3}{6} \right) \right] \end{aligned} \quad (5.213)$$

$$\begin{aligned} \Delta P_{b(x)} &= \Delta P_{b(0)} - b x F_{b(0)} - b x \Delta P_{b(x)} \left(\frac{W L_p}{b \varnothing_{(x)}} \right)^{0.5} \\ &+ b x \Delta P_{b(0)} \left(\frac{W L_p}{b \varnothing_{(x)}} \right)^{0.5} \end{aligned} \quad (5.214)$$

$$\begin{aligned} F_{b(x)} &= F_{b(0)} - \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right) x \Delta P_{b(0)} \right] + \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right) b F_{b(0)} \left(\frac{x^2}{2} \right) \right] \\ &+ \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{0.5} \Delta P_{b(x)} \left(\frac{x^2}{2} \right) \right] \\ &- \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{0.5} \Delta P_{b(0)} \left(\frac{x^2}{2} \right) \right] \end{aligned} \quad (5.215)$$

The volumetric permeated flow rate can be correlated in the form of:

$$\begin{aligned} F_{p(x)} &= F_{p(0)} + \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right) \times \Delta P_{b(0)} \right] - \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right) b F_{b(0)} \left(\frac{x^2}{2} \right) \right] \\ &- \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{0.5} \Delta P_{b(x)} \left(\frac{x^2}{2} \right) \right] + \left[\left(\frac{W L_p}{\varnothing_{(x)}} \right)^{1.5} b^{0.5} \Delta P_{b(0)} \left(\frac{x^2}{2} \right) \right] \end{aligned} \quad (5.216)$$

5.6.14.2 Parameter Estimation

Al-Obaidi et al. (2017f) used the equations of Srinivasan et al. (2010) to predict the unknown parameters of the model and which include L_p , ω , B_s , σ , and b . Model results confirmed that L_p varies between 1.56E-6 and 1.0E-6 m/atm s, ω varies between 0.1E-6 and 1.9E-6 kmol/m² s atm, B_s varies between 0.566E-6 and 1.9E-6 m/s, b varies between 12,826 and 13,537 atm s/m⁴, and σ is 0.9 (dimensionless) for five different inlet feed concentrations. The results of the parameter estimation method are given in Table 5.24.

TABLE 5.24
Results of Parameter Estimation

No.	$C_{b(0)} \times 10^3$	$C_{b(0)}$	T_b	$P_{b(0)}$	$L_p \times 10^6$	$\omega \times 10^6$	$B_s \times 10^6$	B
1	2.125	32.5	4.93	1.56	0.15	1.85	13,006	
2	2.125	33.1	6.90	1.39	0.13	1.89	13,042	
3	2.125	33.0	8.90	1.39	0.10	1.90	13,487	
4	2.125	33.2	10.9	1.43	0.20	1.81	13,537	
5	2.125	34.0	14.8	1.26	0.29	1.13	12,913	
6	4.25	32.2	4.93	1.46	0.54	1.28	13,008	
7	4.25	32.8	6.90	1.34	0.22	1.38	13,039	
8	4.25	33.5	8.90	1.34	1.03	0.83	13,487	
9	4.25	33.9	10.9	1.27	0.35	0.57	13,516	
10	4.25	34.5	12.8	1.26	1.90	1.10	12,867	
11	4.25	34.5	14.8	1.27	1.33	1.17	12,914	
12	6.375	32.5	4.93	1.43	0.10	0.84	13,005	
13	6.375	33.0	6.90	1.16	1.90	0.93	13,030	
14	6.375	33.2	8.90	1.14	0.31	1.06	13,461	
15	6.375	33.5	10.9	1.04	0.24	0.88	13,479	
16	6.375	33.8	12.8	1.07	0.10	0.87	12,839	
17	6.375	34.0	14.8	1.15	1.05	0.62	12,881	
18	8.50	32.0	4.93	1.41	0.11	1.31	13,003	
19	8.50	32.5	6.90	1.22	0.28	1.40	13,027	
20	8.50	32.8	8.90	1.20	0.16	1.40	13,465	
21	8.50	33.0	10.9	1.22	1.37	1.23	13,475	
22	8.50	33.2	12.8	1.15	0.11	1.14	12,844	
23	8.50	33.5	14.8	1.19	0.56	1.12	12,900	
24	10.6	31.5	4.93	1.17	1.90	1.09	12,985	
25	10.6	32.2	6.90	1.11	1.90	1.17	13,009	
26	10.6	32.6	8.90	1.14	0.10	1.08	13,480	
27	10.6	32.8	10.9	1.13	0.11	1.08	13,485	
28	10.6	32.8	12.8	1.00	0.26	1.01	12,826	
29	10.6	33.0	14.8	1.09	1.82	0.85	12,863	

$\sigma = 0.9$

(Adapted from Al-Obaidi et al., 2017f)

5.6.14.3 Model Validation

The predicted values of the model by Al-Obaidi et al. (2017f) were compared with the experimental data of Srinivasan et al. (2010) for the removal of phenol from diluted aqueous solutions at operating feed flow rate of 3.333E-4 m³/s. Figures 5.22 to 5.26 depict this comparison for different operating conditions of phenol rejection,

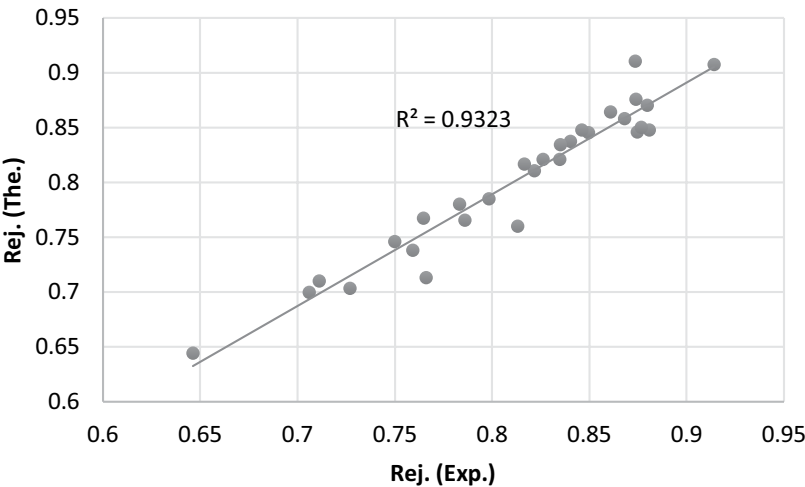


FIGURE 5.22 Comparison of theoretical and experimental results of phenol rejection. (Adapted from Al-Obaidi et al., 2017f)

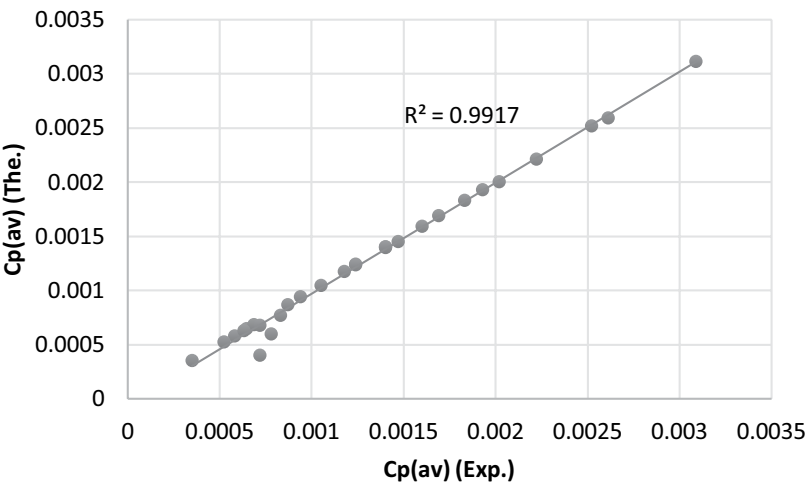


FIGURE 5.23 Comparison of theoretical and experimental results of the average permeate concentration. (Adapted from Al-Obaidi et al., 2017f)

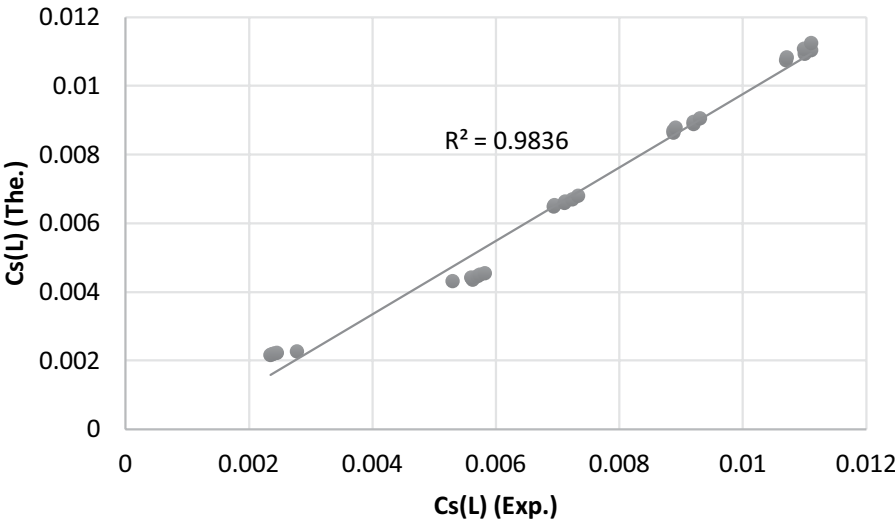


FIGURE 5.24 Comparison of theoretical and experimental results of retentate phenol concentration.
(Adapted from Al-Obaidi et al., 2017f)

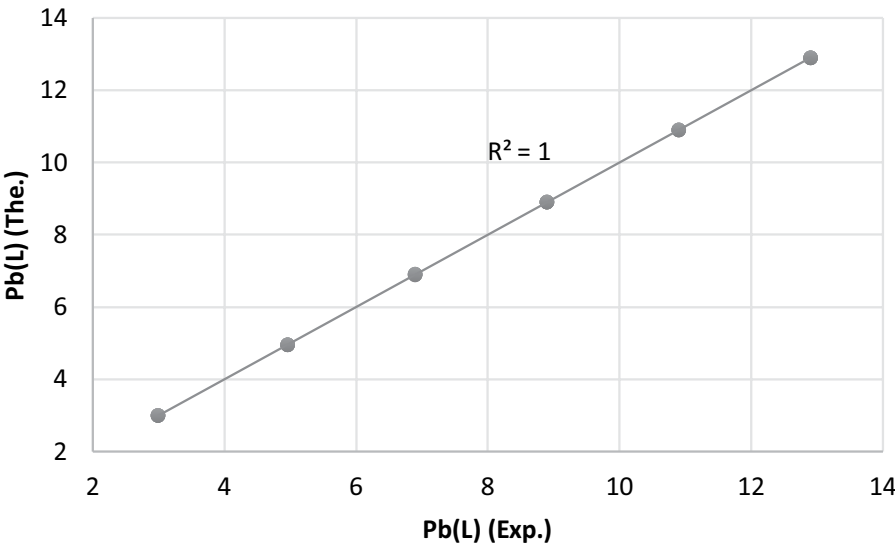


FIGURE 5.25 Comparison of theoretical and experimental results of retentate pressure.
(Adapted from Al-Obaidi et al., 2017f)

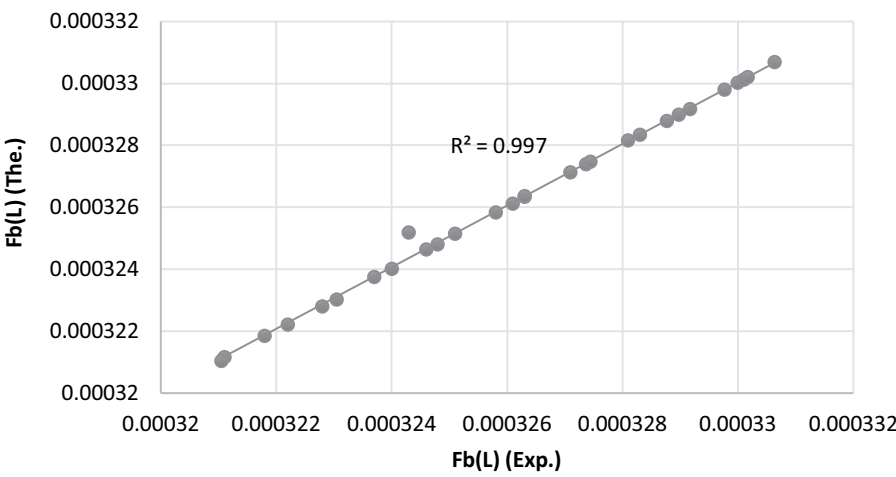


FIGURE 5.26 Comparison of theoretical and experimental results of the retentate flow rate. (Adapted from Al-Obaidi et al., 2017f)

average phenol permeate concentration, retentate phenol concentration, retentate pressure, and retentate flow rate. The model developed yields values very close to the experimental data.

5.7 CRITIQUE ON THE MODELLING OF SPIRAL WOUND REVERSE OSMOSIS PROCESS FOR WASTEWATER TREATMENT

The following observations can be made in respect of the model developed in earlier sections:

- It is evident that there has been no attempt to explore a three-dimensional distributed spiral wound RO process model used especially for wastewater treatment and which handles the investigation of operating parameters as well as their impact along the membrane length, width, and depth.
- The models developed have not considered the fouling impact on the process performance despite the low concentration of pollutants in wastewater. The incorporation of a fouling parameter can ultimately enhance the model prediction of the process rejection and recovery rate, especially when using the high-concentration wastewater for a long time of operation.
- Sagne et al. (2009) have only considered the solute–solute interaction in the treatment of a multiple solutes system using spiral wound RO process. However, this model ignored the concentration polarisation, which provides motivation for developing an improved model.

5.8 CONCLUSIONS

We hope that this chapter has confirmed the appropriateness of the RO process as an effective method for treating secondary effluents at low cost. With the increasing application of RO for the removal of organic compounds, the modelling of membrane separation and mass transport mechanisms constitutes a significant factor in the development of cost-effective and optimum design strategies.

This chapter has confirmed the maturity of several models for removing organic compounds from wastewater using a spiral wound RO process. Many are based on the solution-diffusion and irreversible thermodynamic models. This chapter has provided a one-stop-shop critical appraisal of all the underlying models and associated concepts as well as areas for potential improvement.

This chapter has more specifically provided the state of the art of lumped and distributed parameter models developed in the last decade and associated performance of wastewater treatment methods using the spiral wound reverse osmosis process for the removal of high-toxic organic compounds. The chapter has also included a review of experimental work carried out to remove specific pollutants from wastewater, and such work was used to validate the theoretical models developed.

One of the main conclusions of this chapter is that there is still room for improvement in the prediction, especially for fouling conditions. The predictions of these models for different operating conditions compare favourably to experimental data gathered from the literature for several organic compounds. The models developed can be easily extended for testing other pollutants by simply embedding the physical properties of the relevant pollutants into the model. This chapter has also highlighted the effectiveness of parameter estimation methods used to predict the unknown parameters of the underlying mathematical models. More specifically, the usefulness of the parameter estimation gEST tool available in the gPROMS suite has been highlighted. The purpose of the mathematical modelling of the RO process is to provide a simulation and optimisation tool that can be used to achieve the most effective system design. This chapter has provided the state of the art of such mathematical model concepts for a variety of spiral wound RO process used in wastewater treatment. It has also highlighted the advantages, conceptual differences, and limitations of the models developed.

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6 RO Steady State and Dynamic Simulations for Wastewater Treatment

6.1 INTRODUCTION

The use of RO for treating water and removing several harmful organic compounds has become popular because of its relative ease of use and reduced costs. Several applications have confirmed RO as an efficient separation method for removing both organic and non-organic chemicals found in seawater and wastewater. This chapter showcases such applications for removing highly toxic compounds from wastewater. It also presents the state of the art for both steady state and dynamic RO simulations developed for wastewater treatment and discusses, more particularly, the important impact of several operating parameters on process performance.

6.2 THE IMPORTANCE OF SIMULATION STUDIES

Simulation studies based on theoretical models have been widely used to investigate the hydrodynamics of the RO process. The successful models developed are the ones which can predict the impact of the variation of operating conditions in both axial and spiral directions in respect of operation time. Several steady state and dynamic models have been developed to study the hydrodynamics and transport phenomena of water and solute through the membrane. Such models differ in complexity, rigour, and the underlying assumptions.

RO steady state simulation has several merits. Firstly, it can help both designers and operators understand the contribution of each parameter of the model to process performance. Secondly, it can help determine the specific operating conditions which would yield higher water flux and membrane rejection. Thirdly, it provides a structured solution for optimising one or many objective functions of the process.

RO dynamic simulation also has several merits. Firstly, it can readily be used to analyse process performance indicators when unexpected disturbances in operating conditions occur. Secondly, it can help formulate the development of appropriate control strategies for maintaining a constant performance level. Thirdly, it can help build sufficient evidence for improved confidence when scaling up the process.

6.3 OVERVIEW OF STEADY STATE AND DYNAMIC SIMULATIONS OF RO WASTEWATER TREATMENT

Water flux deterioration during an RO filtration process is mainly due to the accumulation of solute at the membrane surface, which causes an increase in the osmotic pressure of the feed and concentration polarisation. Remedial actions can be taken by modifying the operating conditions, including feed pressure, concentration, temperature, and flow rate. On the other hand, there are factors that can have a positive impact on the RO process, and these include turbulence, back flushing/washing, and pulsed flow.

The performance of RO process is heavily dependent on the operating parameters. A detailed investigation of these parameters and their influence on process responses, such as solute rejection and water recovery, is therefore very important. The outcome of these investigations would be the formulation of the optimum operating conditions, which would yield maximum rejection of pollutants and water recovery.

Several studies can be found in the literature which have attempted to analyse the effects of operating parameters on the performance of individual and multi-stage RO processes given a range of different operating conditions and pollutants.

Chai et al. (1997) studied the impact of operating pressure and temperature on the rejection of copper from synthesised wastewater using two spiral wound RO membranes connected in series. They used the solution-diffusion model (Chapter 5, section 5.4.1) for their study. Simulation results confirmed a linear relationship between the operating pressure and permeate flux. They found that increasing the feed temperature from 34 °C to 40 °C had insignificant impact on permeate concentration.

Mohsen-Nia et al. (2007) confirmed the possibility of achieving more than 98% of copper and nickel removal in a model solution of both pollutants using an individual spiral wound RO process. They used the solution-diffusion model of Lonsdale et al. (1965) (see section 5.4.1) in their study. The larger ion size of copper had marginally increased the overall pollutants rejection, with a positive relationship versus the applied pressure.

The influence of operating parameters on phenol rejection from aqueous solutions has been estimated by Tabassi et al. (2014), based on the Spiegler and Kedem model (Chapter 5, section 5.4.2). In this study, a laboratory-scale spiral wound RO thin-film composite membrane type SG 2514TF of 0.6 m² area from GE Osmonics was used to conduct the filtration process. Simulation results showed that increasing the operating pressure and feed concentration would improve phenol rejection.

The rejection of aqueous solutions of bisphenol using a low-pressure polyamide RO membrane type TW30–1812–100 (Dow FilmTec) of 0.446 m² effective area has been studied by Khazaali et al. (2014). A sensitivity analysis was carried out using the Spiegler, Kedem, and Katchalsky model (Kedem and Katchalsky, 1958, 1963; Spiegler and Kedem, 1966) (described in Chapter 5, section 5.4.2) to explore the effect of operating pressure, flow rate, and concentration on process performance. This study concluded that the increase in feed pressure and flow rate aided bisphenol rejection. More importantly, the study identified critical values of operating pressure and flow rate, which yielded maximum bisphenol rejection. However, this decreased

with an increasing feed concentration, despite low bisphenol rejection at low feed concentration.

Al-Bastaki (2004) used Model I (Chapter 5) in their simulation and reported that a significant improvement of permeate recovery can be achieved as a result of increasing pressure for the removal of methyl orange dye and Na_2SO_4 salt from wastewater using spiral wound RO process. Moreover, a slight increase of salt rejection was noticed due to an increasing feed salt concentration from 500 to 1000 ppm for all the tested operating pressures between 10 and 40 atm.

Ahmad et al. (2007) studied the efficiency of an RO process for treating a multicomponent system of palm oil mill effluent using Model II (Chapter 5) in their simulation. This included the implementation of a wide range of operating pressures and their impacts on water flux and solutes rejections. The unsteady state simulation of several constituents was presented, and these confirmed the improvement of water flux and solute rejection due to elevating operating pressure. This study also concluded that increasing the molecular weight could enhance the solute rejection based on the size exclusion theory.

Sagne et al. (2009) used Model III (described in Chapter 5) to confirm the impact of feed pressure on the removal of five organic solutes from wastewater using RO process. This encompassed the improvement of solute rejection due to increasing transmembrane pressure. The effects of molecular size and solute sorption were used to explain the significant differences of solute rejections.

Comprehensive experimental and modelling research was carried out by Srinivasan et al. (2009, 2010) (using the Model IV described in Chapter 5) to study the effect of the operating conditions on the removal of dimethylphenol and phenol from wastewater, respectively, using a pilot scale of an individual spiral wound RO process. It was clear from this study that increasing the operating pressure could improve dimethylphenol and phenol rejections. However, the pollutant concentration at the permeate channel increased when the feed concentration increased.

The removal of several solutes of the N-nitrosamine family from wastewater has been experimentally investigated by Fujioka et al. (2014) using a pilot scale of three and seven spiral wound modules connected in a series configuration. They also carried out a simulation using Model VI, described in Chapter 5, which showed a significant impact of operating pressure on rejection and water flux. It was observed that increasing the operating temperature would significantly decrease the removal of N-nitrosamine compounds. This can be explained by the impact of temperature on membrane pore size (Sharma et al., 2003). However, the influence of a wider range of operating parameters on process performance was not comprehensively studied by Fujioka et al. (2014).

Extensive simulation studies have been carried out by Al-Obaidi and Mujtaba (2016), Al-Obaidi et al. (2017a, 2017b, 2017c, 2017d) and Al-Obaidi et al. (2018a, 2018b) using different models presented in Chapter 5. Such studies were used to explore the impact of a wide range of operating parameters on the spiral wound RO process for the removal of several phenolic and N-nitrosamine compounds from wastewater. The next sections discuss several successful steady state and dynamic simulations of individual and multi-stage RO process used for the removal of several highly toxic pollutants from wastewater.

6.4 STEADY STATE SIMULATION: SENSITIVITY ANALYSIS OF THE OPERATING PARAMETERS

This section presents a detailed discussion of published steady state simulation studies, including particularly the effect of operating parameters on the performance of the RO process.

6.4.1 REMOVAL OF COPPER FROM ELECTROPLATING WASTEWATER IN TWO RO MEMBRANES

Chai et al. (1997) used a spiral wound RO pilot plant containing two non-cellulose composite membranes connected in series of 10 m² of total membranes area to treat electroplating wastewater containing copper. Figure 6.1 shows the schematic diagram of the RO plant. The steady state simulation is carried out using the solution-diffusion model originally developed by Lonsdale et al. (1965) (Chapter 5, section 5.4.1).

The impact of transmembrane pressure drop on permeate flux and concentration at fixed feed concentration is shown in Figures 6.2 and 6.3 for different temperatures. Figure 6.2 shows a linear relationship between pressure and water flux. It also shows an increase of water flux with the operating temperature. The increase of the membrane water permeability constant with temperature can explain the cause of this phenomenon. A permeate concentration beyond 15 kpa of operating pressure is increased due to increasing the rate of solute flux through the membrane (Figure 6.3). The permeate concentration registered a value below 4 ppm for an original feed concentration of 112 ppm, which signifies copper rejection of around 96.5%.

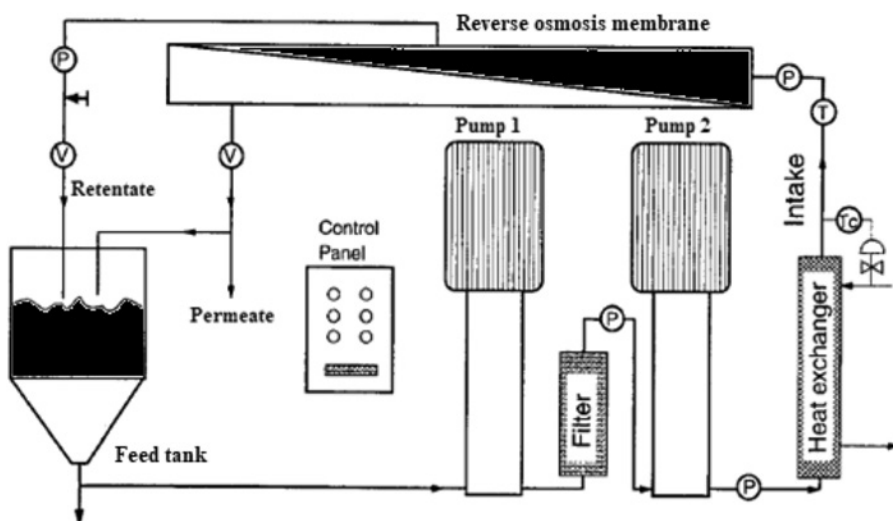


FIGURE 6.1 Schematic diagram of RO process.

(Adapted from Chai et al., 1997)

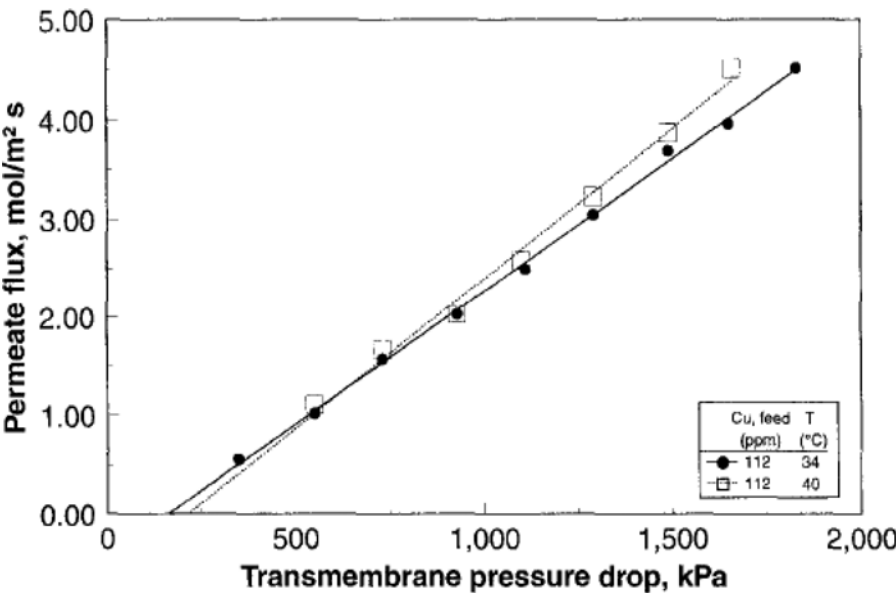


FIGURE 6.2 Permeate flux against transmembrane pressure drop at different feed temperatures.

(Adapted from Chai et al., 1997)

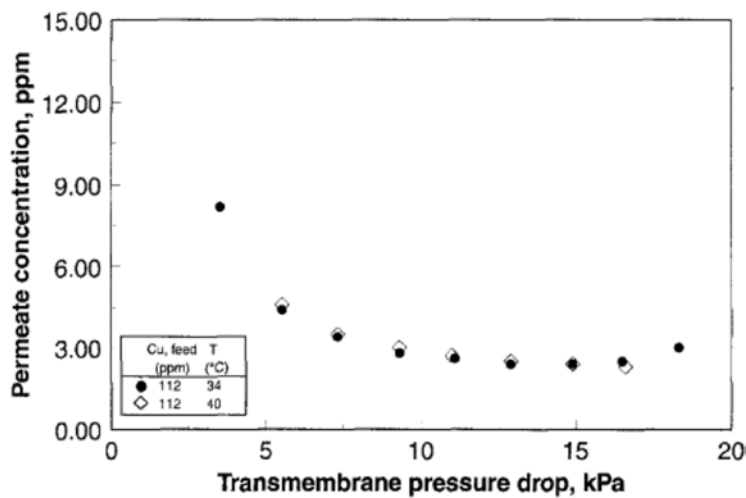


FIGURE 6.3 Permeate concentration against transmembrane pressure drop at different feed temperatures.

(Adapted from Chai et al., 1997)

6.4.2 REMOVAL OF COPPER AND NICKEL FROM WASTEWATER
IN A LABORATORY-SCALE RO PROCESS

Mohsen-Nia et al. (2007) investigated the performance of a laboratory-scale RO process of an individual spiral wound module containing a thin-film composite polyamide membrane type (RE2012–100) manufactured by CSM of 1.95 m². This was used to treat synthetic wastewater containing a mixed system of copper Cu⁺² and nickel Ni⁺² of 500 ppm. Figure 6.4 shows the schematic diagram of the corresponding RO process. Lonsdale et al. (1965) (Chapter 5, section 5.4.1) was used to estimate the permeate concentration and the overall rejection of both pollutants. Results confirmed a linear positive relationship between the applied pressure and the high values of copper and nickel rejections of more than 98% (Figure 6.5). It was also noticed

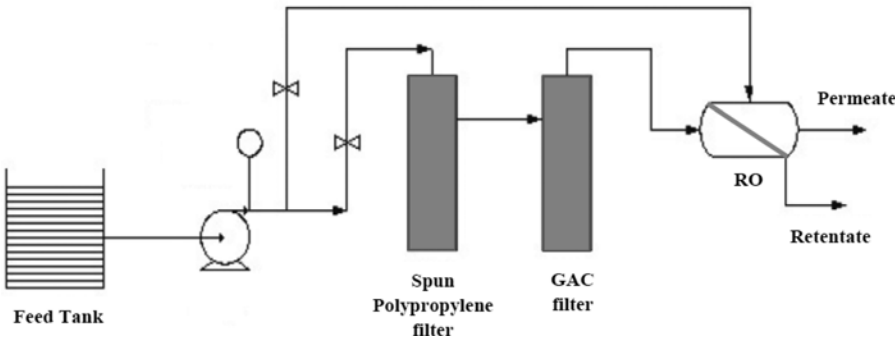


FIGURE 6.4 Schematic diagram of RO process.

(Adapted from Mohsen-Nia et al., 2007)

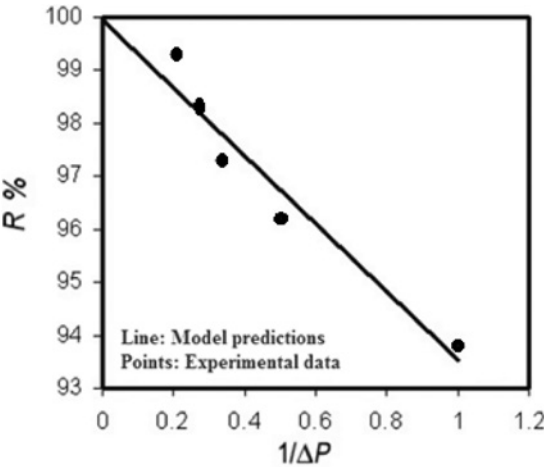


FIGURE 6.5 Experimental data and model predictions of overall copper and nickel rejection against the reciprocal of pressure.

(Adapted from Mohsen-Nia et al., 2007)

that increasing the feed concentration of copper in the mixed system of 500 ppm would insignificantly increase the overall rejection. This is ascribed to a bigger ion size of copper compared to that of nickel.

6.4.3 REMOVAL OF METHYL ORANGE DYE AND Na_2SO_4 SALT FROM WASTEWATER USING SPIRAL WOUND RO PROCESS

Al-Bastaki (2004) studied the performance of an individual spiral wound RO process of membrane type FilmTec SW30 (2.1 m² of surface area) for the removal of methyl orange dye ($\text{C}_{14}\text{H}_{14}\text{N}_3\text{NaO}_3\text{S}$) and Na_2SO_4 salt from wastewater using the Model I described in Chapter 5. The influence of increasing the operating pressure from 10 atm to 40 atm on the removal of Na_2SO_4 salt from wastewater and permeate recovery with no dye added is shown in Figure 6.6 at 10,000 ppm feed concentration. This study confirmed insignificant increase of salt removal and significant increase of recovery as a result of increasing pressure. The same insignificant trend of methyl orange dye removal is concluded and presented in Figure 6.7.

It was also noticed that the synthesised wastewater containing both salt and dye exhibiting an increasing dye concentration of 500 to 1000 ppm caused a slight reduction in the permeate recovery. More importantly, the removal of salt was not considerably increased due to increasing the dye concentration from 500 to 1000 ppm at 5000 ppm salt concentration, as clearly shown in Figure 6.8.

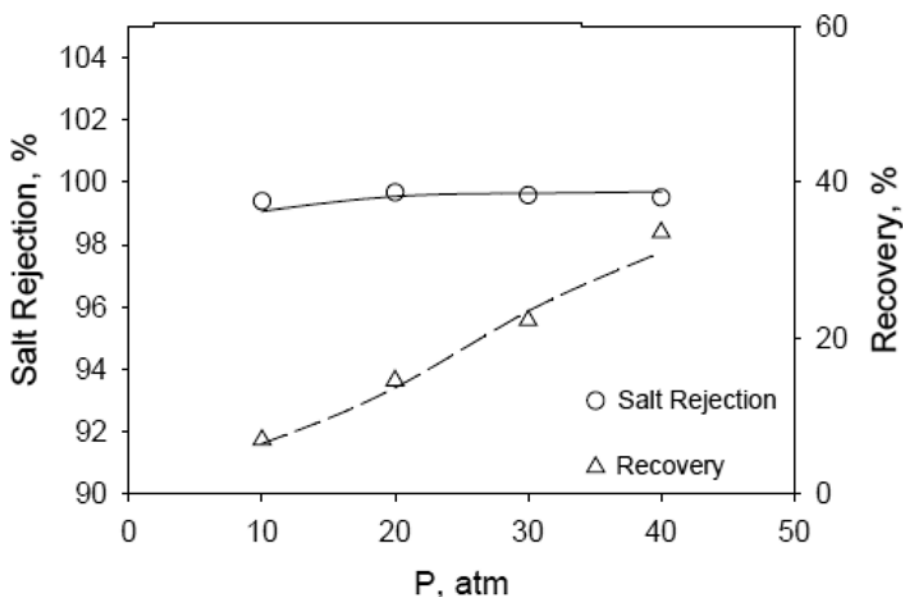


FIGURE 6.6 Influence of feed pressure on Na_2SO_4 salt rejection and permeate recovery with no dye added.

(Adapted from Al-Bastaki, 2004)

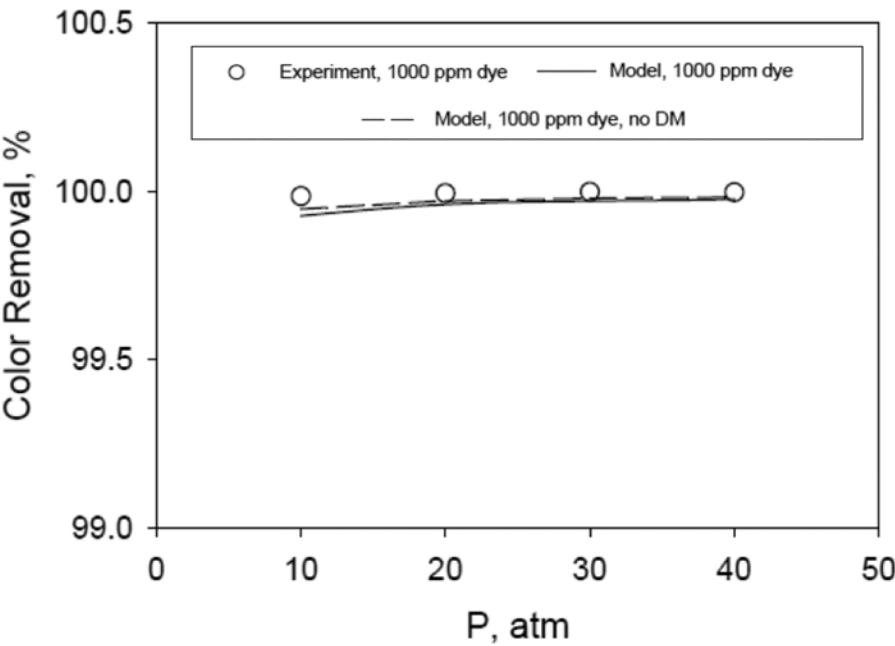


FIGURE 6.7 Influence of feed pressure on dye removal with no salt added.
(Adapted from Al-Bastaki, 2004)

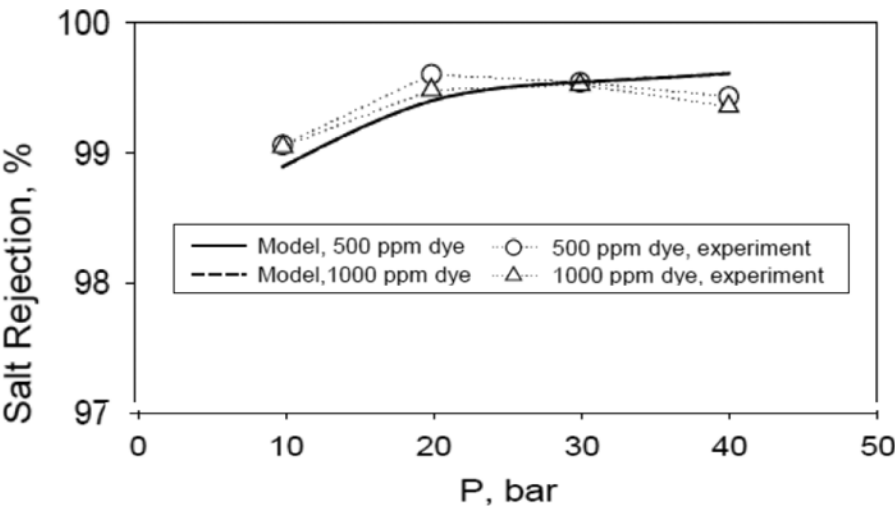


FIGURE 6.8 Influence of dye concentration on salt removal of binary solution.
(Adapted from Al-Bastaki, 2004)

6.4.4 REMOVAL OF TERNARY SOLUTES FROM PALM OIL MILL EFFLUENTS USING RO PROCESS

Ahmad et al. (2007) carried out an experimental study to investigate the efficiency of a pilot-scale RO membrane system (0.9 m² of an effective area) to treat pretreated palm oil mill effluent (POME) at room temperature of 25 °C. The POME contained a ternary system of carbohydrate constituents, protein, and ammoniacal nitrogen solutes.

This study analysed the impact of increasing the feed pressure from 13.5 bar to 45 bar at constant feed flow rate and solute concentrations along the operating time on the permeate recovery. This showed a significant increase of water flux due to increasing the transmembrane pressure as presented in Figure 6.9. Also, the simulation results (using Model II of Chapter 5) showed that increasing the feed pressure would increase the fractional wall concentrations for each solute. This explained an improvement of the intrinsic solute rejection as a result of increasing the feed pressure (Figure 6.10).

The study also concluded that increasing the higher molecular weight of solutes could help improve the removal efficiency of carbohydrate constituents and protein observed. Results show this at a higher rate than those for ammoniacal nitrogen, which are of lower molecular weight.

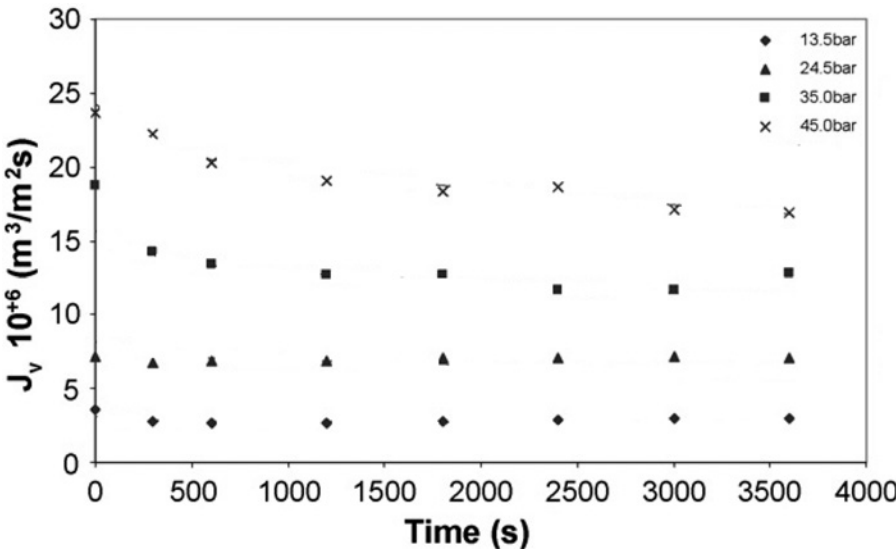


FIGURE 6.9 Impact of feed pressure on water flux at fixed solutes concentrations, flow rate, and temperature.

(Adapted from Ahmad et al., 2007)

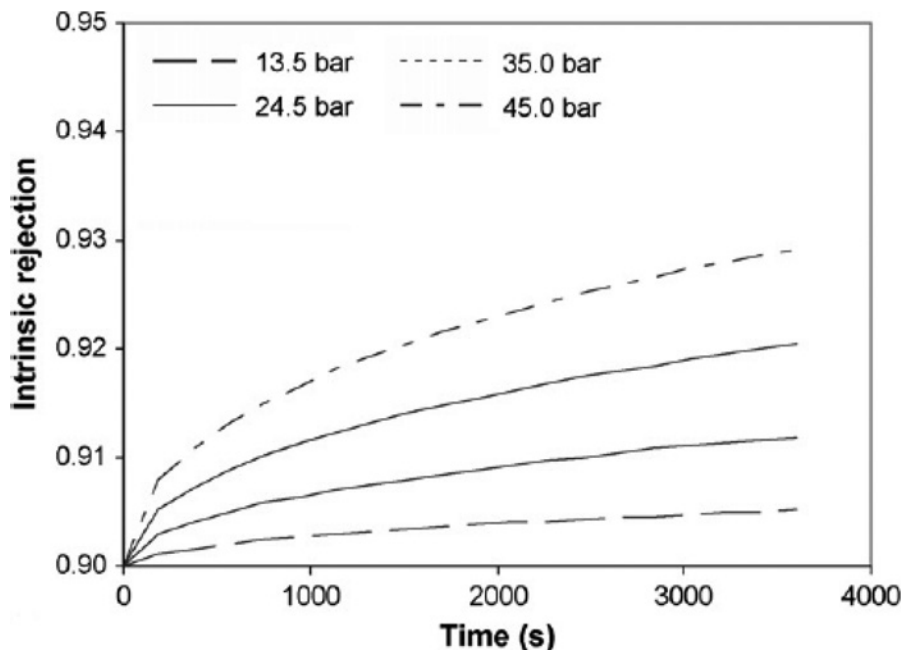


FIGURE 6.10 Impact of feed pressure on intrinsic unsteady state rejection of carbohydrate constituents.

(Adapted from Ahmad et al., 2007)

6.4.5 REMOVAL OF VOLATILE ORGANIC MOLECULES FROM WASTEWATER USING RO PROCESS

Sagne et al. (2009) studied the impact of different operating pressures of 5, 10, 15, 20, and 30 bar on the solute rejections of volatile organic molecules and permeate flux at steady state conditions of spiral wound RO process. This included a permeate and retentate recycling mode into the feed tank (batch experiments). The synthetic mixture of the five solutes of acetic acid, butyric acid, furfural, 2-phenylethanol, and 2,3-butanediol was considered. The simulation results (using Model III of Chapter 5) confirmed a permeate flux increase due to increasing the pressure. Moreover, the solute rejection increased as a result of increasing the pressure, where there were lower rejections of both acetic acid and furfural as compared with butyric acid, 2-phenylethanol, and 2,3-butanediol (Figure 6.11). This is mainly attributed to their physico-chemical characteristics, size effect, and sorption properties.

6.4.6 REMOVAL OF PHENOL FROM WASTEWATER IN SG RO MEMBRANE

Tabassi et al. (2014) used a commercial thin-film composite RO membrane spiral wound type SG 2514TF (made by GE Osmonics) to remove phenol from wastewater.

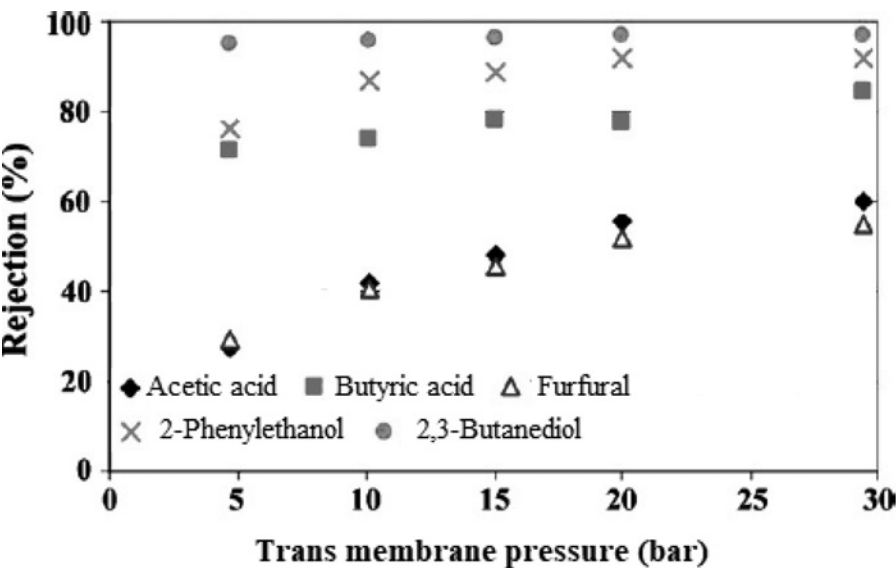


FIGURE 6.11 Impact of transmembrane pressure on solute rejection.
(Adapted from Sagne et al., 2009)

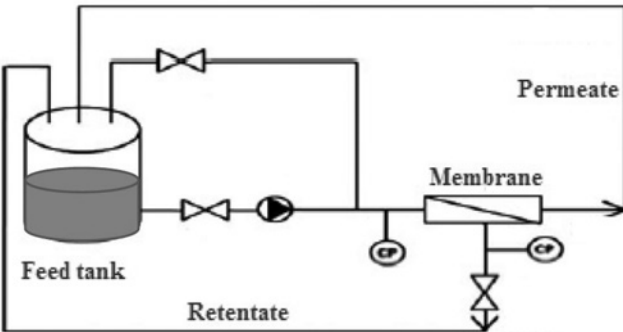


FIGURE 6.12 Schematic diagram of RO process.
(Adapted from Tabassi et al., 2014)

The impact of several operating conditions was investigated in respect of water flux and phenol retention. The Spiegler and Kedem (1966) model (Chapter 5, section 5.4.2) was used to quantify the water convection and phenol diffusion through the membrane. Figure 6.12 shows a schematic diagram of the RO process.

The impact of transmembrane pressure was analysed on phenol retention as shown in Figure 6.13. This shows a progress of retention against the applied pressure. It is not surprising to notice an increase in water flux as a response to an increasing

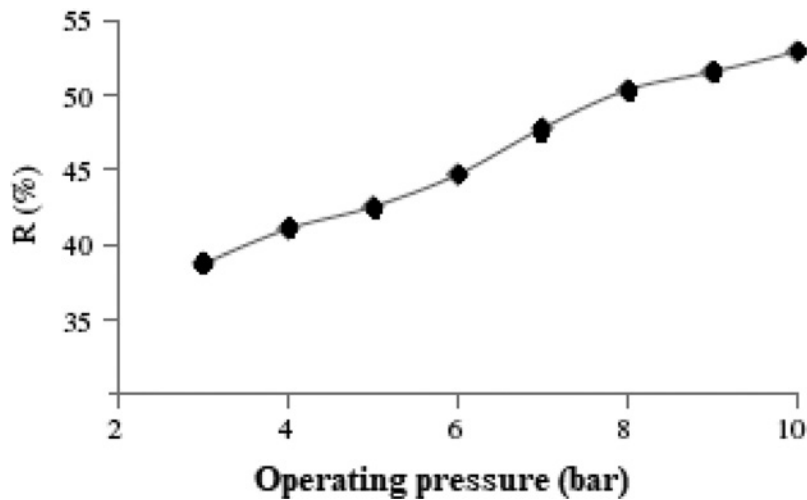


FIGURE 6.13 Applied pressure against phenol rejection (operating conditions: 50 ppm and 6.5 pH).

(Adapted from Tabassi et al., 2014)

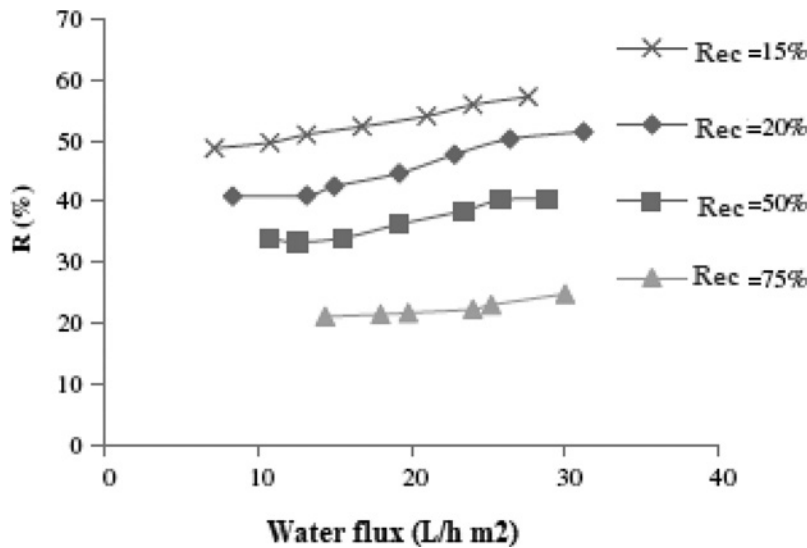


FIGURE 6.14 Permeate flux against phenol rejection at different water recovery (operating conditions: 50 ppm and 6.5 pH).

(Adapted from Tabassi et al., 2014)

feed pressure, which would increase the rate of dilution of permeate concentration in the permeate channel. It was also noticed that the recovery rate of RO membrane can be increased by reducing the crossflow along the membrane feed channel. However, any increase in water recovery would consequently reduce the retention of

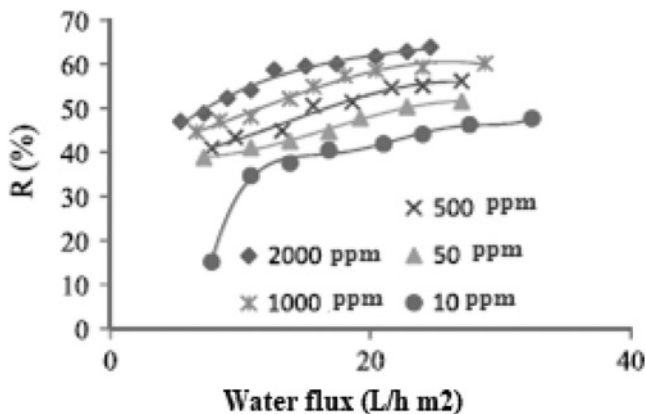


FIGURE 6.15 Permeate flux against phenol rejection at different feed concentration (operating conditions: Rec 20%, and 6.5 pH).

(Adapted from Tabassi et al., 2014)

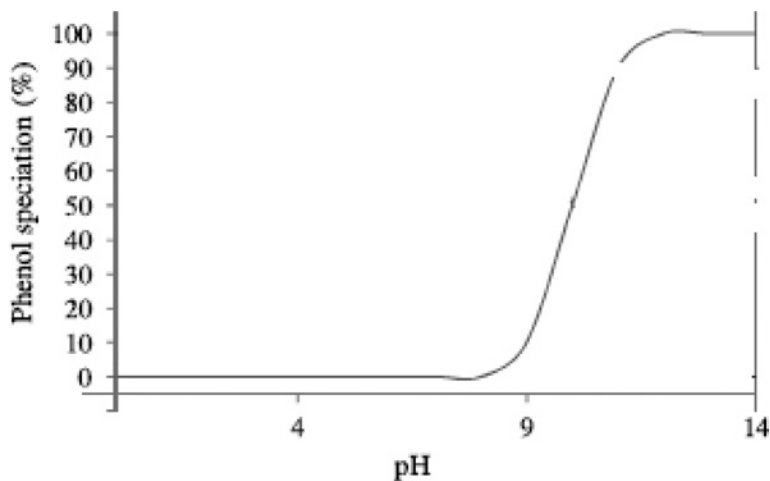


FIGURE 6.16 Fluid pH against phenol retention (operating conditions: 50 ppm, 7 bar, Rec 20%).

(Adapted from Tabassi et al., 2014)

phenol as depicted in Figure 6.14, which illustrates the variation of permeate flux and water recovery on phenol retention. This shows a reduction of phenol retention as a response to increasing the recovery rate, which is systematically attained by reducing the crossflow velocity. The net effect of this is an increase of the growth of phenol at the membrane surface and an increase of the solute flux.

The effect of feed concentration on phenol rejection is shown in Figure 6.15, with an increase of retention due to increasing phenol concentration. This is attributed to the low increase in phenol concentration at the permeate channel compared to the increase in bulk phenol concentration in the feed channel. Figures 6.16 and 6.17

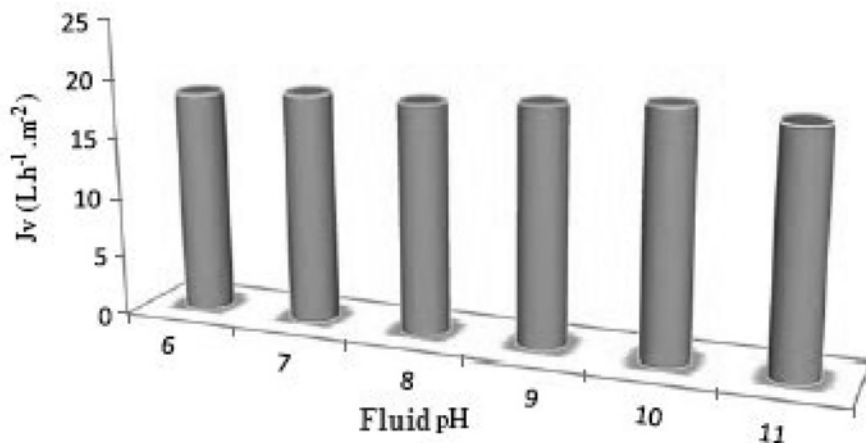


FIGURE 6.17 Permeate flux against fluid pH (operating conditions: 50 ppm, 7 bar, Rec 20%).

(Adapted from Tabassi et al., 2014)

show that the fluid phenol retention is dependent on pH, unlike water flux. The phenol has low retention at acidic and neutral mediums. However, the phenol retention reaches 90% at a pH higher than 9. This is caused by the increase in concentration of dissociated phenolic ion and the growth of the negatively charged solutes. The net effect of this is an increase of the electrostatic repulsion with the negatively charged membrane surface.

6.4.7 REMOVAL OF BISPHENOL A FROM WASTEWATER IN LOW-PRESSURE RO PROCESS

Khazaali et al. (2014) investigated the effect of several operating conditions on the removal of bisphenol A from aqueous waste using an RO process of a low-pressure polyamide thin-film composite membrane type TW30–1812–100 made by Dow FilmTec (0.445 m²). This included the investigation of the optimum conditions for attaining maximum bisphenol retention. Figure 6.18 shows the schematic diagram of the corresponding RO process. Performance indicators were represented using the Spiegler, Kedem, and Katchalsky model (Kedem and Katchalsky, 1958, 1963; Spiegler and Kedem, 1966) developed for an RO membrane.

The influence of feed pressure on bisphenol A retention was investigated at different pHs but at fixed feed flow rate and concentration. The rejection of bisphenol A was increased with increasing pressure with the presence of a critical pressure reaching an optimum rejection followed by a continuous reduction. At this optimum pressure, the bisphenol A concentration at the membrane-feed interface is significantly increased; this causes an increase of solute flux, which in turn reduces the retention value. Figure 6.19 shows that increasing the pH has a passive impact on

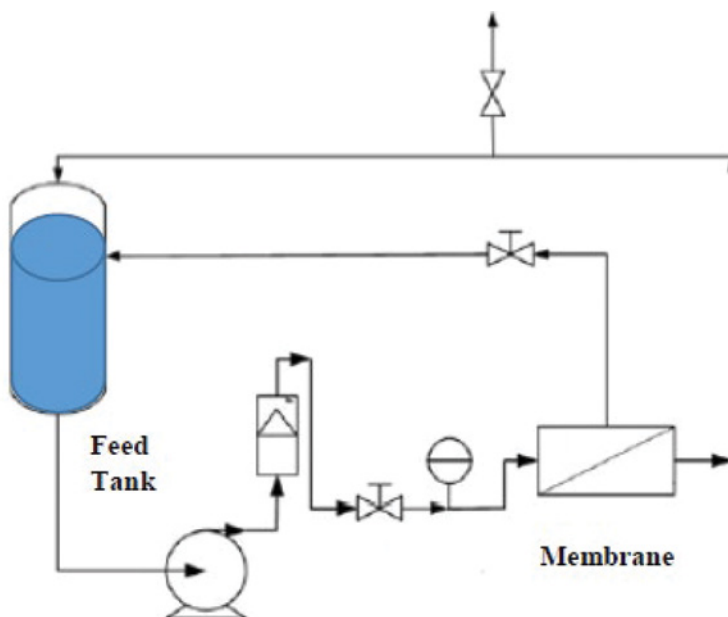


FIGURE 6.18 Schematic diagram of RO process.

(Adapted from Khazaali et al., 2014)

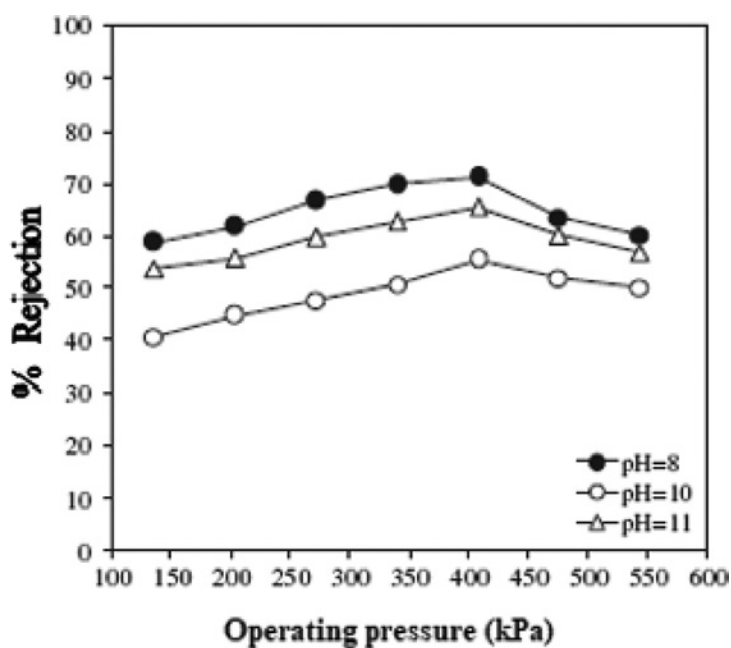


FIGURE 6.19 Operating pressure against bisphenol A rejection at different pH (operating conditions: 1.172 L/min and 30 ppm).

(Adapted from Khazaali et al., 2014)

retention. Interestingly, a minimum rejection is observed at pH = 10. Seemingly, the negative charge of bisphenol A is increased at a pH more than 7, which rises the repulsion with a negatively charged membrane surface. Also, increasing the pH more than 10 was enough to increase the rate of bisphenol A dissociation, which strengthens the retention value.

The effect of feed concentration on bisphenol A rejection at fixed feed flow rate and pH is depicted in Figure 6.20, which shows a continuous reduction due to higher concentration polarisation. In other words, an increase of the feed concentration would increase the osmotic pressure and thus decrease the water flux through the membrane.

Figure 6.21 presents the influence of feed flow rate on bisphenol A rejection at fixed feed concentration and pH. This explains the retention increase due to an increasing feed flow rate. In other words, increasing the crossflow velocity would reduce the thickness of concentration polarisation layer, which in turn decreases the effective osmotic pressure that enhances water flux.

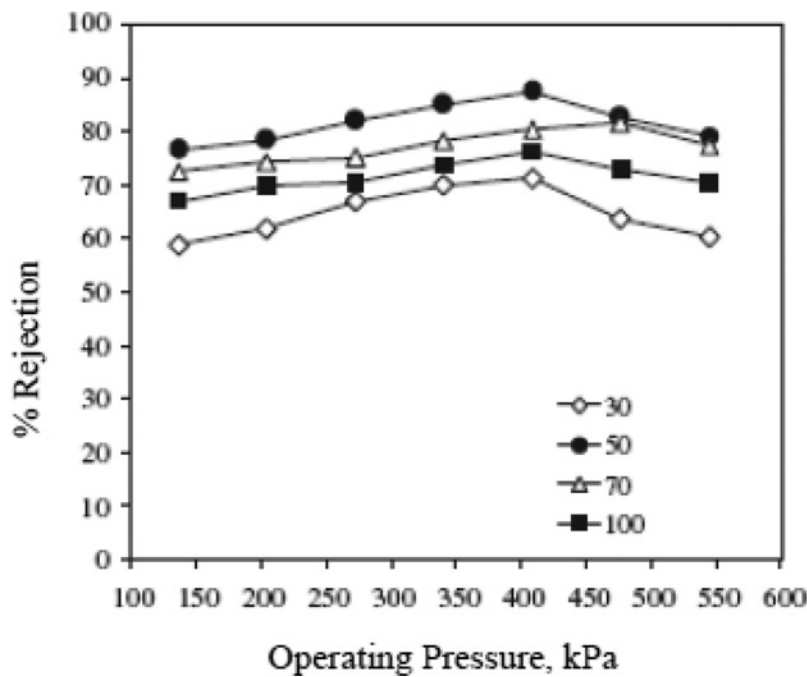


FIGURE 6.20 Operating pressure against bisphenol A rejection at different feed concentrations (operating conditions: 1.172 L/min and pH = 8).

(Adapted from Khazaali et al., 2014)

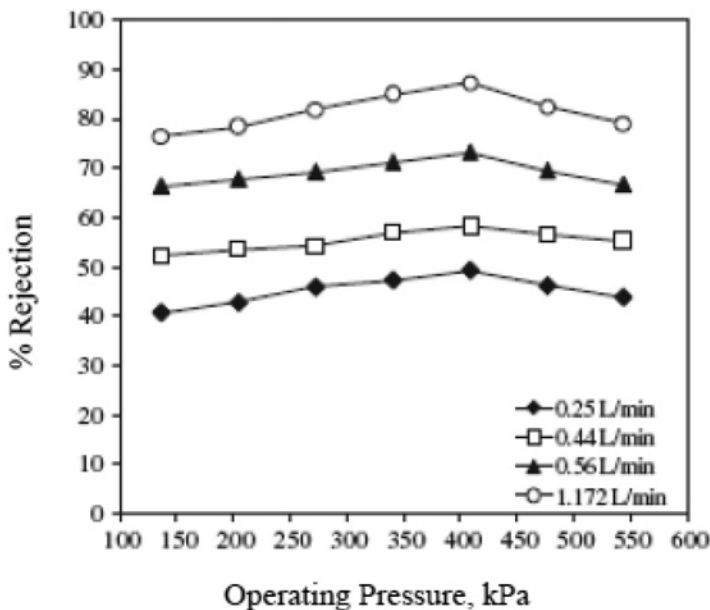


FIGURE 6.21 Operating pressure against bisphenol A rejection at different feed flow rates (operating conditions: 50 ppm and pH = 8).

(Adapted from Khazaali et al., 2014)

6.4.8 REMOVAL OF CHLOROPHENOL FROM WASTEWATER IN AN INDIVIDUAL SPIRAL WOUND RO PROCESS

Chlorophenol is a toxic compound for humans and can readily be found in the effluent of several industrial applications. Specifically, its low concentration can deter the usage of reused water in various industrial applications. The sensitivity analysis carried out in this study used Model VII by Al-Obaidi and Mujtaba (2016) (Chapter 5) for the removal of chlorophenol from wastewater using an individual spiral wound module of RO process, which was described by Sundaramoorthy et al. (2011). Note: Sundaramoorthy et al. (2011) developed Model V as described in Chapter 5. Readers are also directed to the original reference. The impact of several operating conditions on the RO performance was investigated as is described in the next sections.

6.4.8.1 Feed Flow Rate

Feed flow rate and specifically crossflow is a significant parameter in any RO process. It is basically related to the Reynolds number of fluid, which in turn affects the concentration polarisation. In this respect, high crossflow can help the reduction of concentration polarisation due to its high shear stress. Figure 6.22 shows the variation of feed flow rate along the membrane channel. In particular, the reduction of

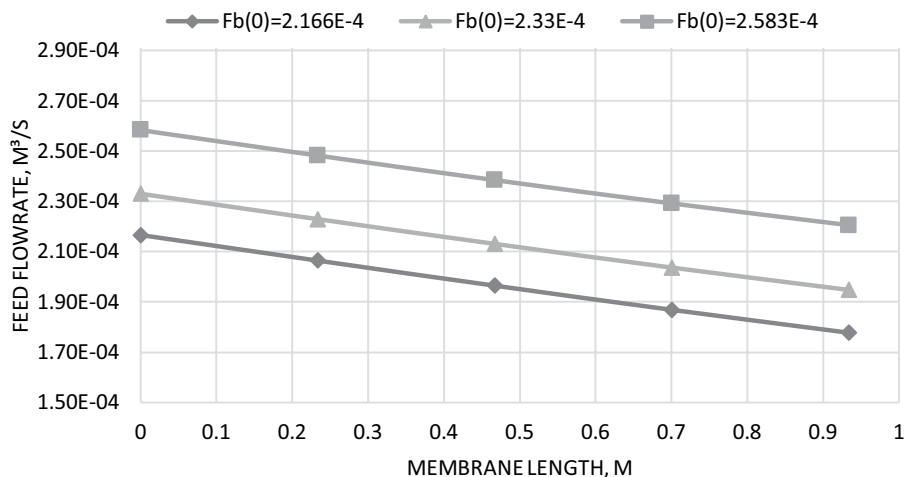


FIGURE 6.22 Steady state feed flow rate along the membrane length of different inlet feed flow rates (inlet feed conditions, $2.335\text{E-}3 \text{ kmol/m}^3$, 7.77 atm, and 32 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

feed flow rate along the membrane channel can be ascribed to the permeate penetrating the membrane because of a high operating pressure. It is therefore reasonable to notice an increasing bulk chlorophenol concentration along the membrane length (Figure 6.23). Essentially, the retention of chlorophenol at the membrane surface with the diffusion of water through the membrane causes the increase of bulk concentration, which lifts the osmotic pressure. Any increase in the feed flow rate would increase the mass transfer coefficient and decrease the concentration polarisation. This in turn has a significant positive impact on the bulk concentration gradient along the membrane length (Figure 6.23). In addition to this, the applied pressure decreases along the membrane length because of the friction between the flowing water and membrane surface (Figure 6.24). This in turn reduces the net pressure of the water flux driving force and therefore brings down the diffusion rate of water (Figure 6.25). Based on this phenomenon, any increase of the applied pressure would increase the water flux by raising the transmembrane pressure above the osmotic pressure.

Figure 6.26 shows the influence of the feed flow rate on the total permeate flux. It would be possible to expect that increasing the feed flow rate would increase the total permeate flux due to the consequential reduction in the concentration polarisation. However, based on the simulation results shown in Figure 6.26, it is evident that increasing the feed flow rate has an insignificant impact on the total permeated flow rate at any operating pressure. This is in line with no decrease of the water flux (Figure 6.27).

Figure 6.27 depicts the possibility of decreasing the concentration polarisation especially in the inlet region of the membrane, where any increase in the feed flow rate would somehow improve the water flux through the membrane. Therefore, the

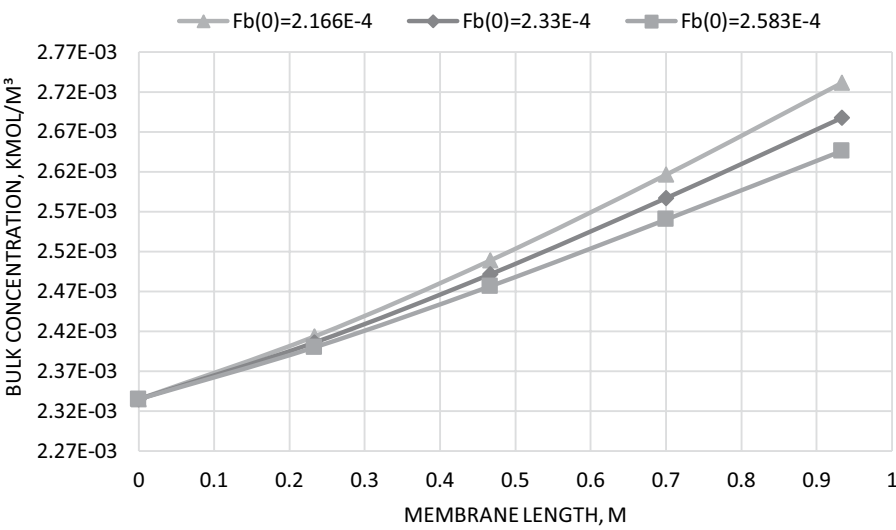


FIGURE 6.23 Steady state feed chlorophenol concentration along the membrane length of different inlet feed flow rates (inlet feed conditions, $2.335\text{E-}3 \text{ kmol/m}^3$, 7.77 atm , and $32 \text{ }^\circ\text{C}$). (Adapted from Al-Obaidi and Mujtaba, 2016)

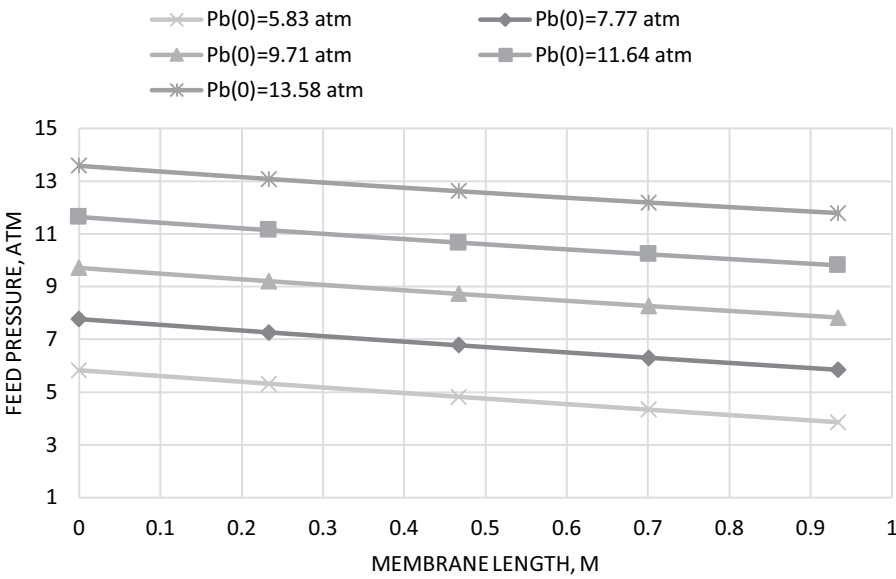


FIGURE 6.24 Steady state water flux along the membrane length of different inlet feed pressures (inlet feed conditions, $2.583\text{E-}4 \text{ m}^3/\text{s}$, $6.226\text{E-}3 \text{ kmol/m}^3$, and $31 \text{ }^\circ\text{C}$). (Adapted from Al-Obaidi and Mujtaba, 2016)

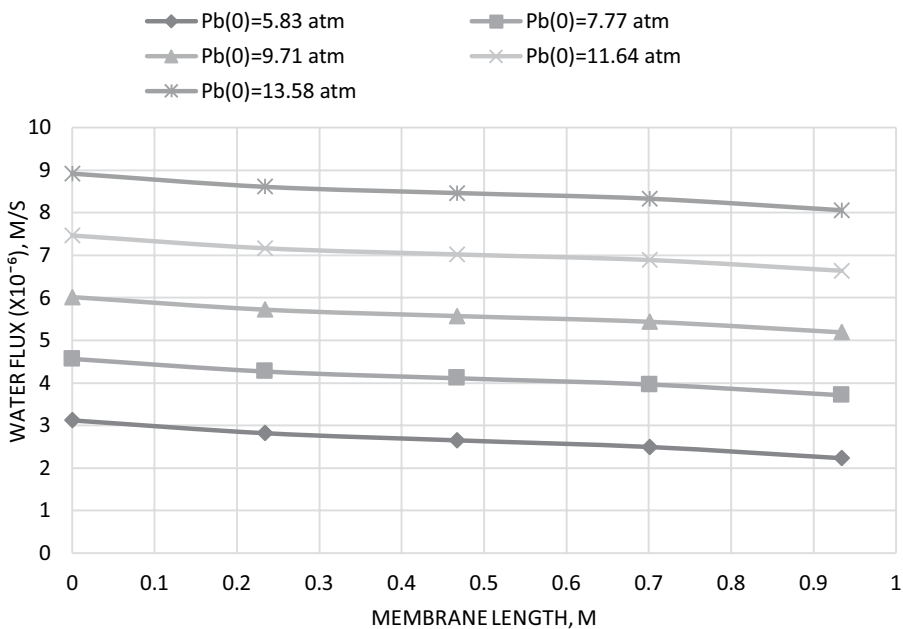


FIGURE 6.25 Steady state water flux along the membrane length for different inlet feed pressures (inlet feed flow rate $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, inlet feed concentration $0.006226 \text{ kmol/m}^3$, and inlet feed temperature 31°C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

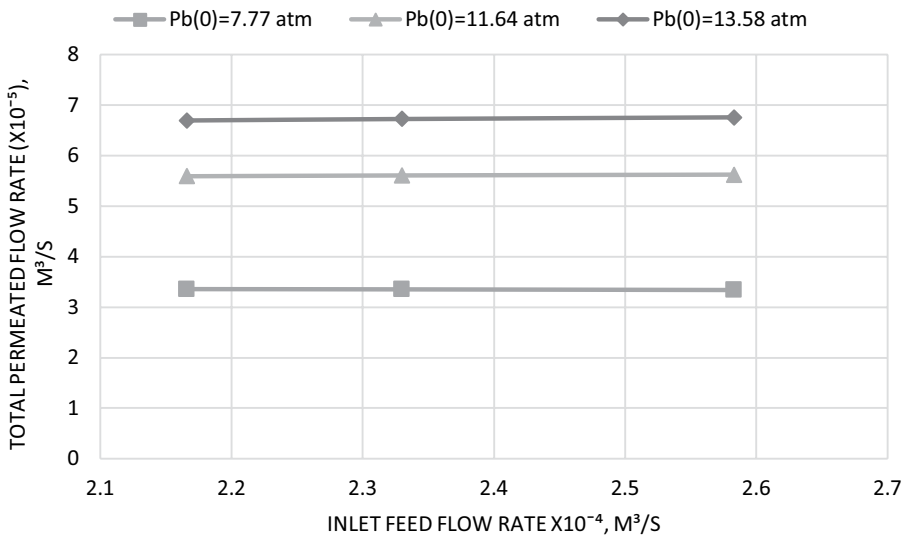


FIGURE 6.26 Steady state total permeated flow rate versus inlet feed flow rate of different inlet feed pressures (inlet feed conditions, $6.226\text{E-}3 \text{ kmol/m}^3$, and 31°C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

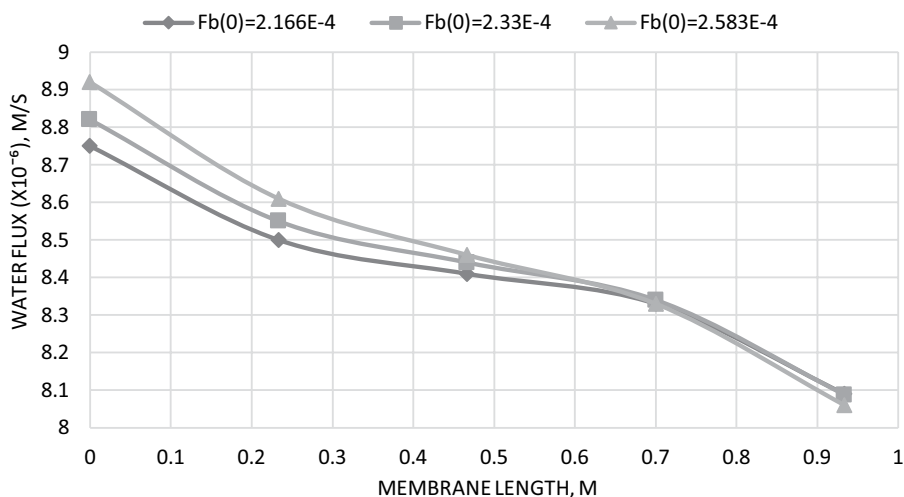


FIGURE 6.27 Steady state water flux along the membrane length of different inlet feed flow rates (inlet feed conditions, 13.58 atm, $6.226E-3$ kmol/m³, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

total water recovery decreases along the membrane length as a result of increasing feed flow rates (Figure 6.28). The slight reduction of total water recovery with increasing feed flow rate can be attributed to two factors. Firstly, increasing feed flow rate causes a high level of friction that results in a frictional pressure drop, which outweighs the gain in osmotic pressure reduction in each point along the membrane length. This would thus reduce the driving force of the water flux. Secondly, increasing the feed flow rate decreases the residence time of feed inside the module, which in turn reduces the quantity of water flux. Also, increasing the operating pressure increases the total water recovery (Figure 6.29). This same observation is also reported in several research studies, including those of Avlonitis et al. (1993) and Abbas (2005).

The influence of increasing the feed flow rate on the permeate chlorophenol concentration at the permeate channel is shown in Figure 6.30. Increasing the inlet feed flow rate reduces the average permeate chlorophenol concentration at the permeate channel despite a small change in the permeated water (Figure 6.26). This is due to the increase of the mass transfer coefficient of chlorophenol because of the increase of the feed flow rate as shown in Figure 6.31. The net effect of this is a decrease of the solute flux in terms of a reduced concentration polarisation and chlorophenol concentration at the membrane surface as shown in Figure 6.32. The outcome of this is a reduction of the permeated concentration of chlorophenol (Figure 6.30). Based on all the aforementioned observations, a slight increase of the solute rejection is expected as a result of increasing the feed flow rate (Figure 6.33). The increase in chlorophenol rejection is explained further in the next section.

Increasing the feed flow rate has a positive influence on the mass transfer coefficient, which reduces the concentration polarisation. However, increasing feed flow

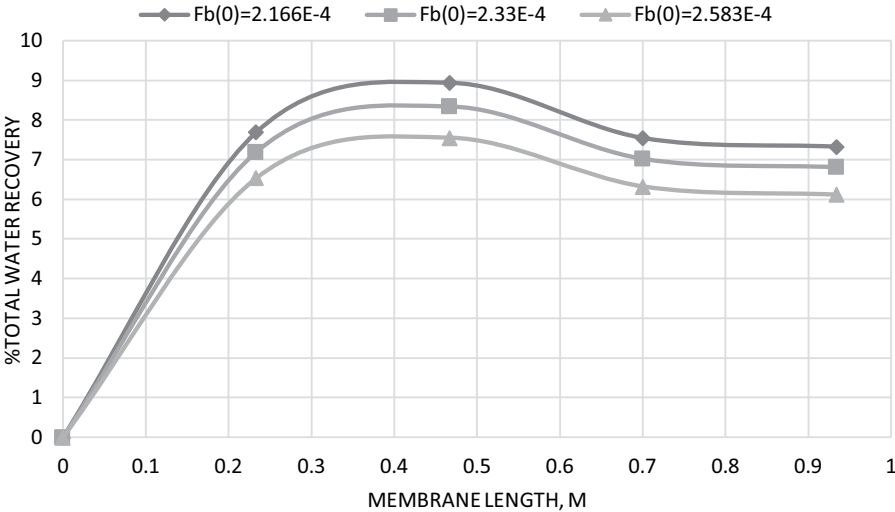


FIGURE 6.28 Steady state total water recovery along the membrane length of different inlet feed flow rates (inlet feed chlorophenol conditions, 6.226×10^{-3} kmol/m³, 13.58 atm, and 31 °C).
(Adapted from Al-Obaidi and Mujtaba, 2016)

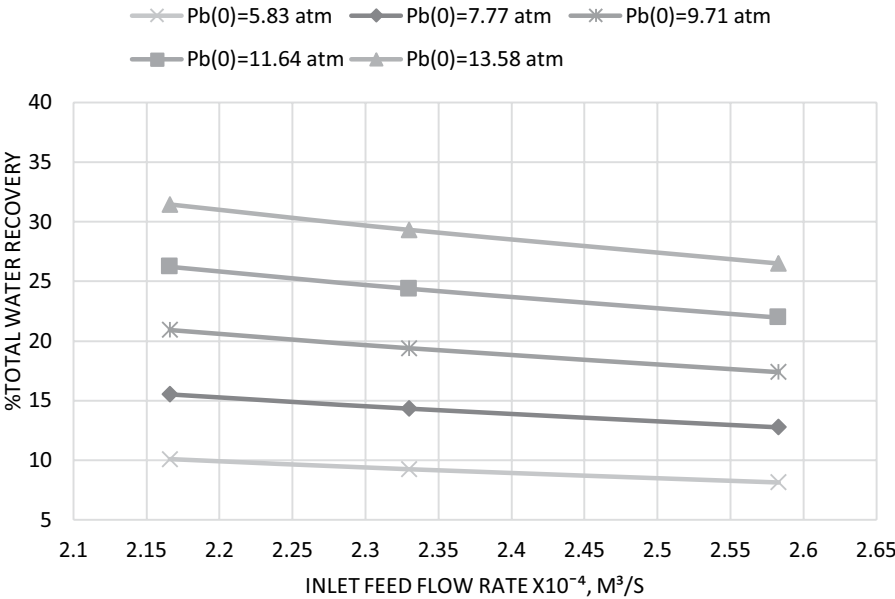


FIGURE 6.29 Steady state total water recovery with the inlet feed flow rate for different inlet feed pressures (inlet feed chlorophenol concentration 0.006226 kmol/m³ and inlet feed temperature 31 °C).
(Adapted from Al-Obaidi and Mujtaba, 2016)

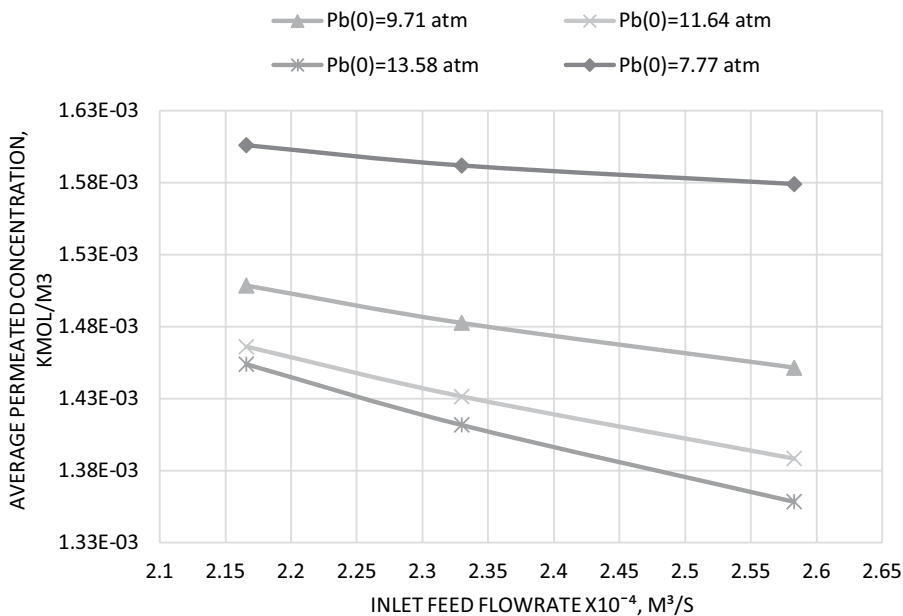


FIGURE 6.30 Steady state average permeated chlorophenol concentration with inlet feed flow rates for different inlet feed pressures (inlet feed concentration $0.006226 \text{ kmol/m}^3$ and inlet feed temperature 31°C)

(Adapted from Al-Obaidi and Mujtaba, 2016)

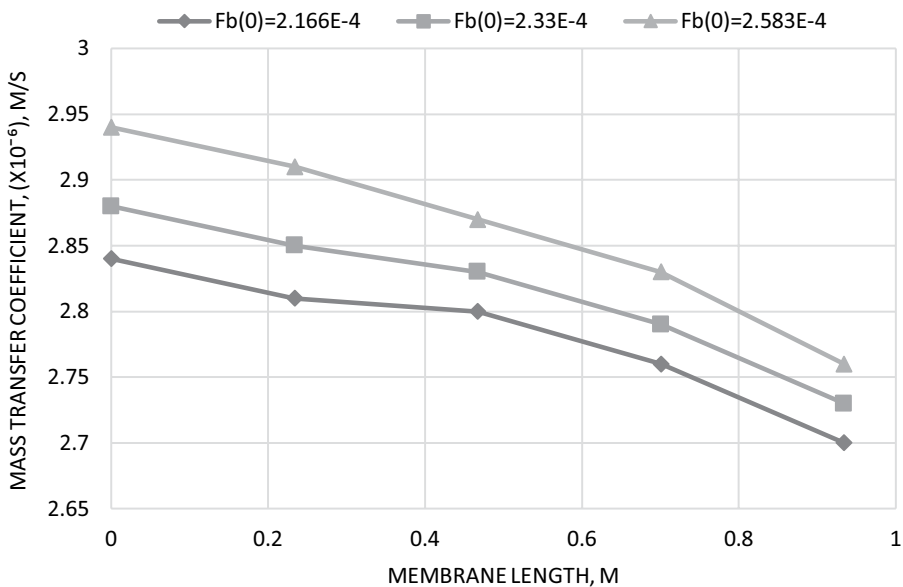


FIGURE 6.31 Steady state mass transfer coefficient along the membrane length for different inlet feed flow rates (inlet feed chlorophenol concentration $0.006226 \text{ kmol/m}^3$, inlet feed pressure 13.58 atm , and inlet feed temperature 31°C)

(Adapted from Al-Obaidi and Mujtaba, 2016)

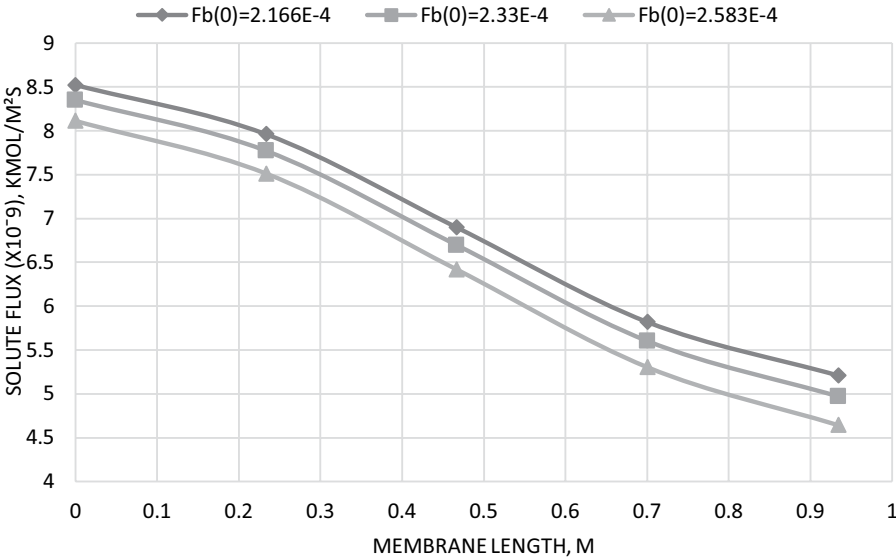


FIGURE 6.32 Steady state solute flux along the membrane length for different inlet feed flow rates (inlet feed chlorophenol concentration 0.006226 kmol/m³, inlet feed pressure 9.71 atm, and inlet feed temperature 31 °C)

(Adapted from Al-Obaidi and Mujtaba, 2016)

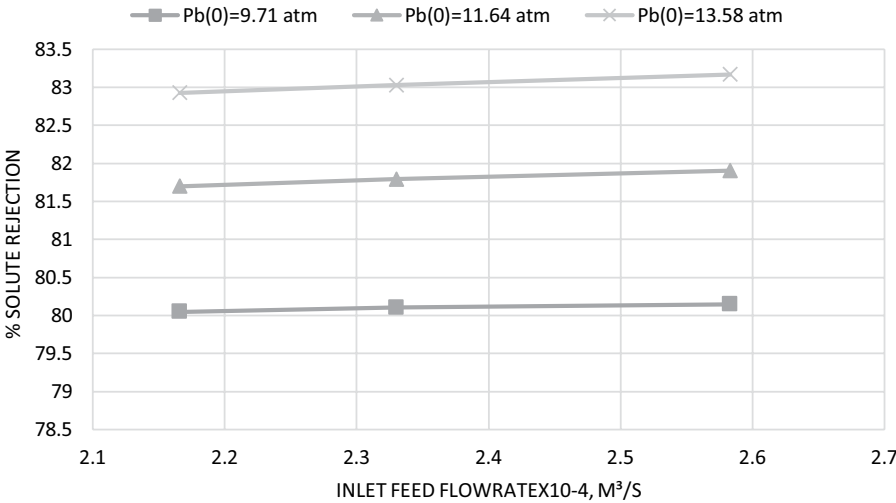


FIGURE 6.33 Steady state chlorophenol rejection versus inlet feed flow rates of different inlet feed pressures (inlet feed chlorophenol conditions, 6.226E-3 kmol/m³, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

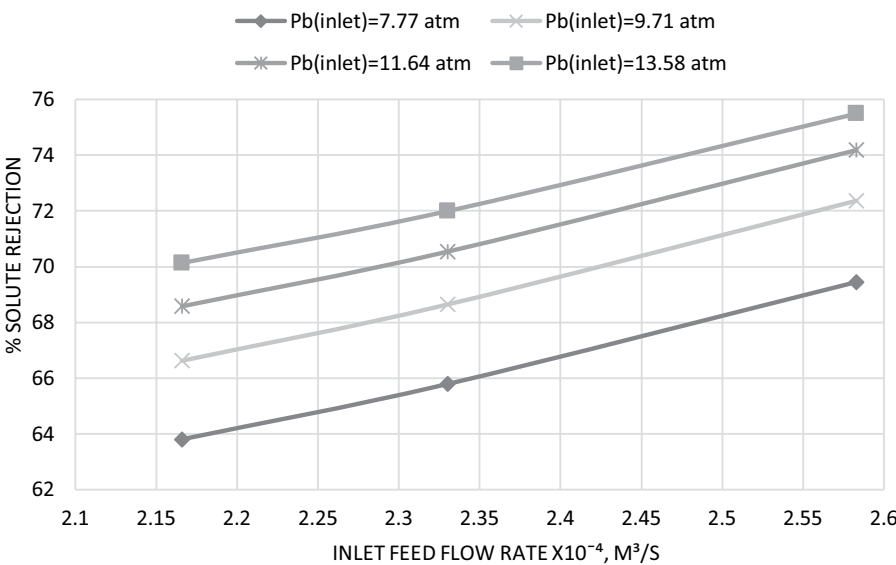


FIGURE 6.34 Steady state chlorophenol rejection versus inlet feed flow rates of different inlet feed pressures (inlet feed conditions, $1.556E-3$ kmol/m³, and 32 °C).
(Adapted from Al-Obaidi and Mujtaba, 2016)

rate causes an increase in the friction, which retards the water flux. This is why the chlorophenol rejection is slightly increased for the operating conditions tested (inlet feed concentration 0.006226 kmol/m³). Figure 6.33 also shows that the rate of increase of chlorophenol rejection is more pronounced at higher feed flowrate and pressure conditions compared to that at low feed flowrate and low pressures. However, at lower feed concentrations of chlorophenol, such as $1.556E-3$ kmol/m³, the chlorophenol rejection increases when the feed flowrate and pressure and the rate of change increase, as more particularly shown in Figure 6.34. This is due to the low impact of concentration polarisation along the membrane length, which inherently improves the mass transfer coefficient and water flux.

In addition, a reduction of the chlorophenol concentration of permeated water is expected when the operating pressure increases due to an increase of the rate of dilution caused by increasing the water flux (Figure 6.30). All the previously mentioned observations are in line with the experimental data of Sundaramoorthy et al. (2011) and clearly demonstrate the suitability of the model for further applications.

6.4.8.2 Operating Pressure

As can be seen from Figure 6.34, the operating pressure has a significant positive impact on chlorophenol rejection. This means that increasing the operating pressure at any concentration results in an enhanced quality of permeate at the permeate channel and a reduced permeate concentration, as more particularly shown in Figure 6.35. It is also expected that increasing the operating pressure at any

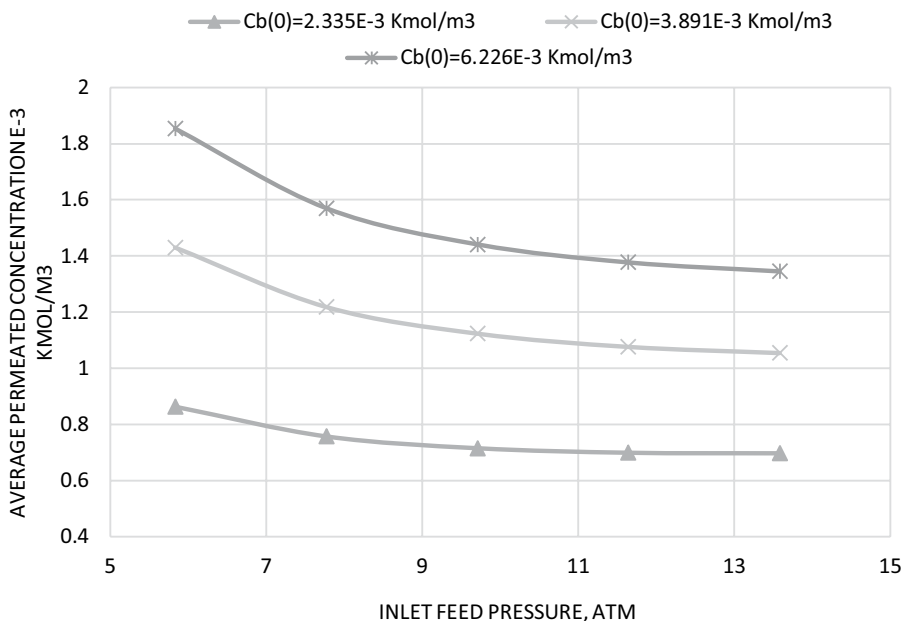


FIGURE 6.35 Steady state average permeate chlorophenol concentration versus inlet feed pressures of different inlet feed chlorophenol concentrations (inlet feed conditions 2.583×10^{-4} m³/s and 32°C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

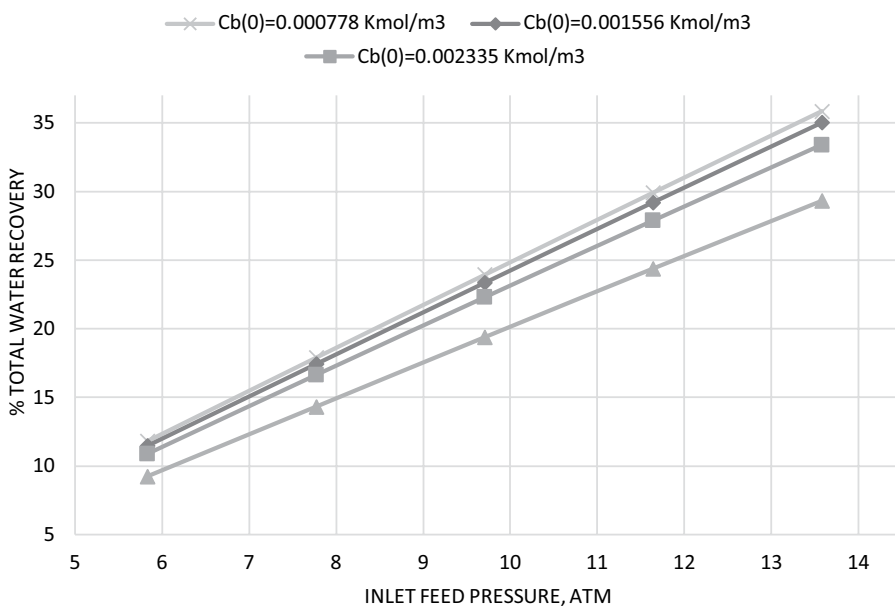


FIGURE 6.36 Steady state total water recovery versus inlet feed pressures of different inlet feed chlorophenol concentrations (inlet feed conditions, 2.583×10^{-4} m³/s, and 32°C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

operating concentration would increase the water flux through the membrane, which would ultimately increase the total water recovery as shown in Figure 6.36. Another conclusion can be made from Figures 6.35 and 6.36 in that any increase in the feed chlorophenol concentration at any operating pressure has a negative impact on both the averages of the permeate concentration and the total water recovery, respectively. This is due to the increasing osmotic pressure and feed concentration, which retard the water flux.

6.4.8.3 Operating Concentration

Figure 6.37 shows the reduction of water flux along the membrane length as a result of increasing the chlorophenol feed concentration. This can be attributed to the increased osmotic pressure, which reduces the driving force for the water flux. These results are consistent with the findings of Kim et al. (2009). However, Figure 6.38 confirms a noteworthy increase of rejection as a result of increasing the feed concentration. This may be attributed to increasing the membrane solute rejection intensity. This is a critical parameter used in this study to investigate the trend of chlorophenol rejection along the membrane length. The membrane solute rejection intensity is given in Eq. (6.1) for each point of the x-axis along the membrane length of feed channel.

$$\% \text{Solute Rejection Intensity} = \frac{C_{b(x)} - C_{p(x)}}{C_{b(x)}} \times 100 \tag{6.1}$$

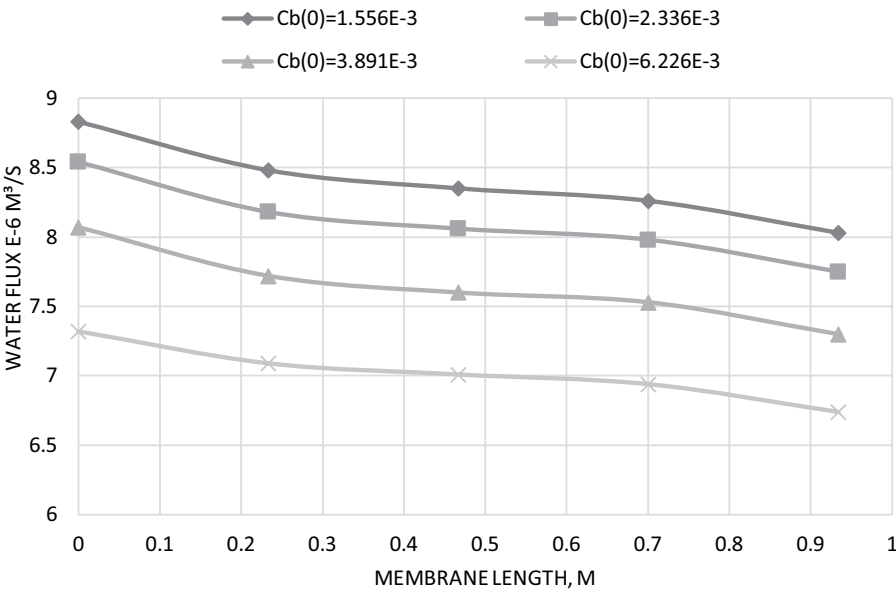


FIGURE 6.37 Steady state water flux along the membrane length of different inlet feed concentrations (inlet feed conditions, 2.166E-4 m³/s, 11.64 atm, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

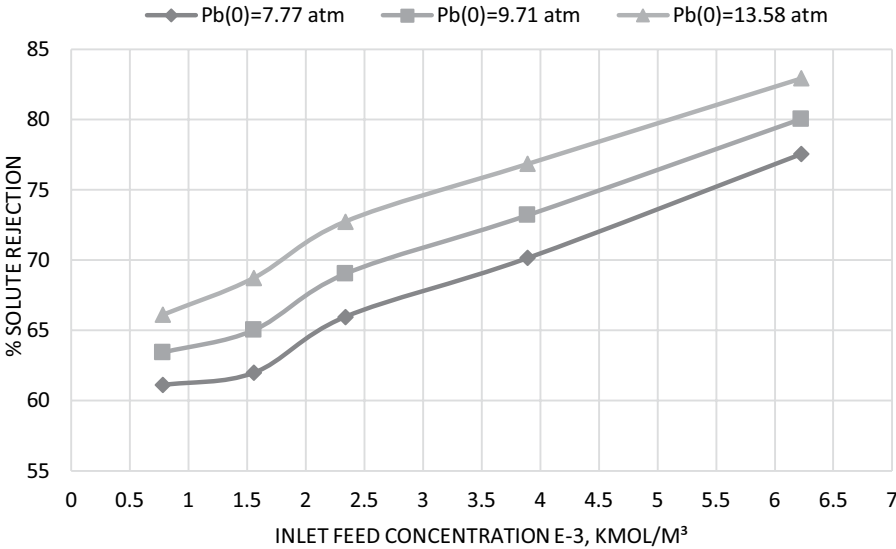


FIGURE 6.38 Steady state solute rejection versus inlet feed concentrations of different inlet feed pressures (inlet feed conditions, 2.166E-4 m³/s, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

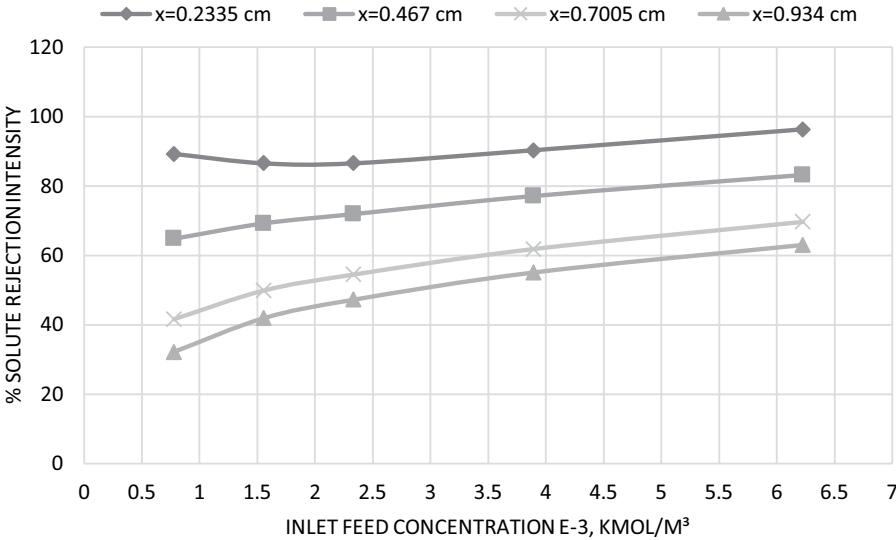


FIGURE 6.39 Steady state membrane solute rejection intensity versus inlet feed concentrations of different points along the membrane length (inlet feed conditions, 2.166E-4 m³/s, 11.64 atm, and 32 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

Figure 6.39 shows the calculation of the membrane solute rejection intensity at several points of the x-axis along the membrane length. This shows a maximum value at the beginning of the membrane and a minimum value at the end of the membrane. More importantly, increasing the operating concentration reinforces the isolation intensity. Avlonitis et al. (1993) affirmed the same observations, highlighting the fact that the operating pressure has essentially a considerable impact on chlorophenol rejection, as depicted in Figure 6.38.

6.4.9 REMOVAL OF DIMETHYLPHENOL FROM WASTEWATER IN AN INDIVIDUAL SPIRAL WOUND RO PROCESS

Dimethylphenol is one of the phenolic organic compounds which can be found in many industrial effluents such as from petroleum processing and disinfectant, herbicide, and plastic manufacturing (Gami et al., 2014).

The experimental work of Srinivasan et al. (2011) for the removal of dimethylphenol from aqueous solutions of different concentrations was used to validate Model VIII (Chapter 5) by Al-Obaidi et al. (2017b).

6.4.9.1 Sensitivity Analysis

Figure 6.40 and Figure 6.41 show the steady state simulation of feed flow rate and pressure based on two dimensions of membrane length and width (x and y axes) of the spiral wound RO process. Figure 6.40 shows a clear decline in the feed flow rate

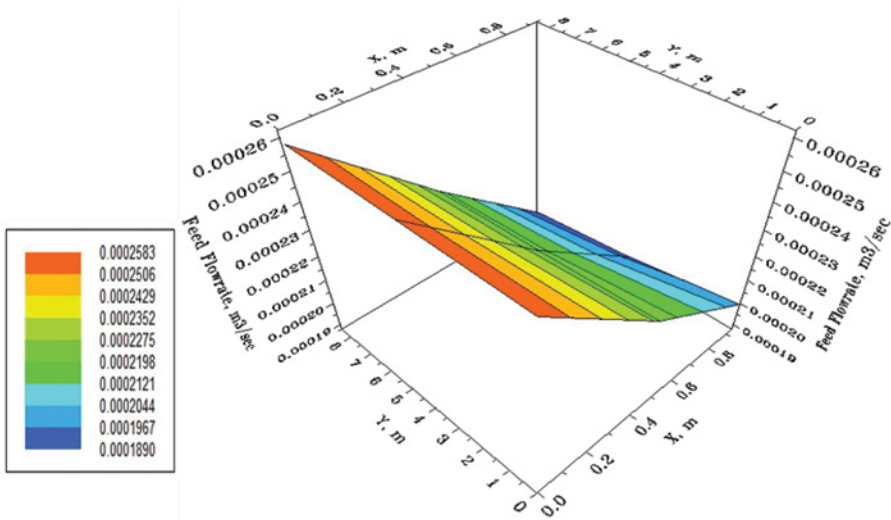


FIGURE 6.40 Feed flow rate in the two dimensions at inlet conditions ($2.583\text{E-}4\text{ m}^3/\text{s}$, $6.548\text{E-}3\text{ kmol}/\text{m}^3$, 13.58 atm, and $31.5\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi et al., 2017b)

as a result of water permeation through the membrane, with a similar drop in the operating pressure. This is illustrated in Figure 6.41 due to the friction in the wall membrane.

Based on the previous observations, it is fair to expect a spatial increase in bulk dimethylphenol concentration at the feed channel as a result of the increasing retention of dimethylphenol along the membrane wall (Figure 6.42). This means a continuous increase in the solute built up on the membrane surface along the membrane length, as shown in Figure 6.43, due to the increased concentration polarisation and osmotic pressure. This reduces the driving force of water flux as shown in Figure 6.44, which depicts an increase of water flux in the y coordinates despite the spatial reduction of water flux in the x coordinate. The simulation results given in Figure 6.41 confirm that higher values of applied pressure, especially at the outlet edge of the membrane width, result in a lower feed flow rate (Figure 6.40) compared to the inlet edge of the membrane width.

Figure 6.45 depicts the response of the solute rejection versus a variation in both feed pressure and concentration of the ranges 5.83 to 13.58 atm and 0.819E-3 to 6.548E-3 kmol/m³, respectively. This simulation is carried out at fixed feed flow rate and temperature of 2.583E-4 m³/s and 31 °C, respectively.

An increase from 88% to 96.8% of dimethylphenol rejection is noticed with changing operating pressure. Moreover, there is a clear increase in the dimethylphenol rejection as a function of the feed concentration, and the increase in water flux and membrane rejection intensity can be attributed to these responses.

The total water recovery can be considered as an important performance indicator of the RO process. Figure 6.46 shows a clear increase in the water recovery when

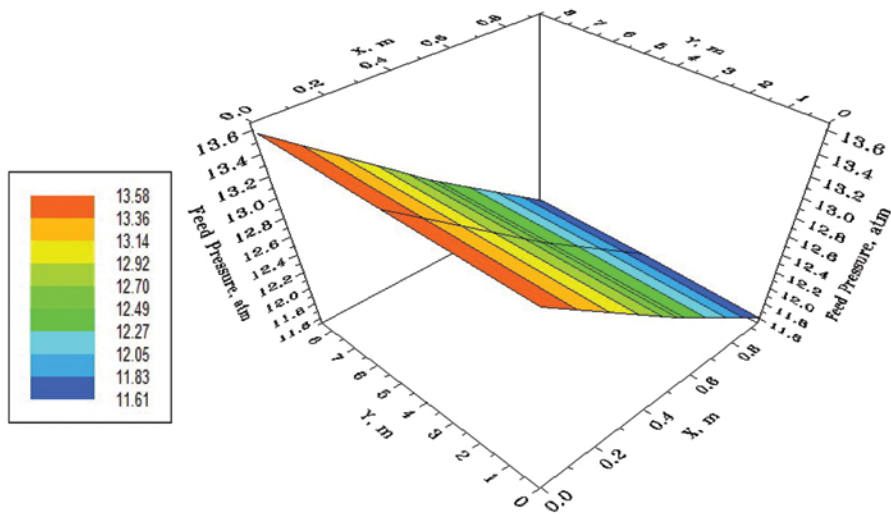


FIGURE 6.41 Feed pressure in the two dimensions at inlet conditions (2.583E-4 m³/s, 6.548E-3 kmol/m³, 13.58 atm, and 31.5 °C).

(Adapted from Al-Obaidi et al., 2017b)

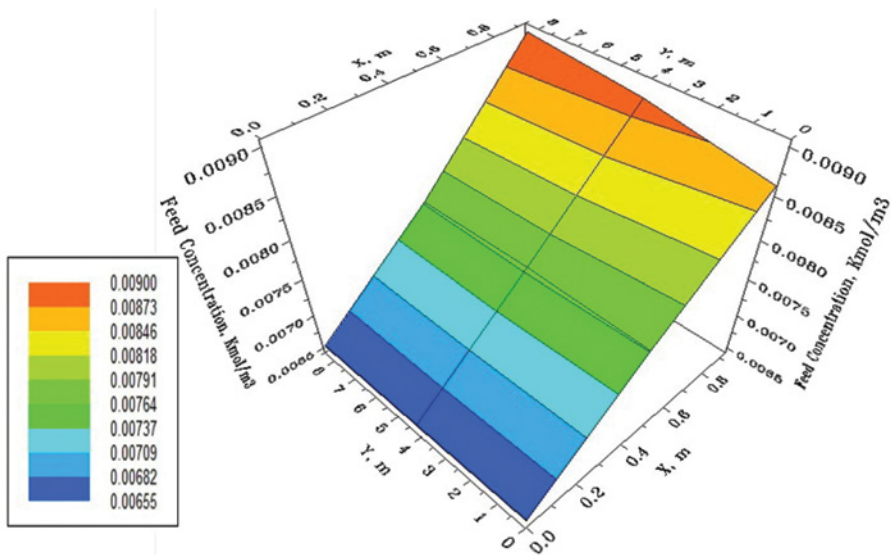


FIGURE 6.42 Feed concentration in the two dimensions at inlet conditions ($2.583\text{E-}4\text{ m}^3/\text{s}$, $6.548\text{E-}3\text{ kmol/m}^3$, 13.58 atm, and $31.5\text{ }^\circ\text{C}$).
(Adapted from Al-Obaidi et al., 2017b)

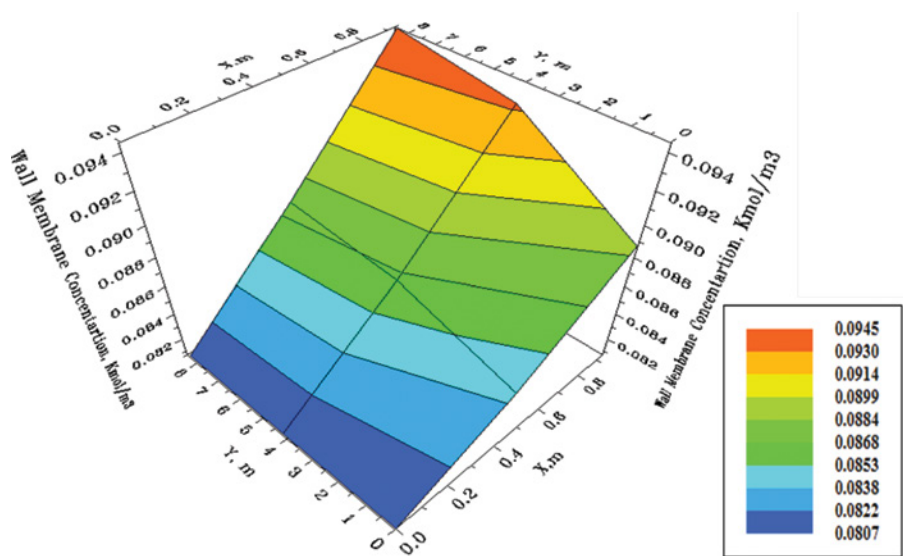


FIGURE 6.43 Wall membrane concentration in the two dimensions at inlet conditions ($2.583\text{E-}4\text{ m}^3/\text{s}$, $6.548\text{E-}3\text{ kmol/m}^3$, 13.58 atm, and $31.5\text{ }^\circ\text{C}$).
(Adapted from Al-Obaidi et al., 2017b)

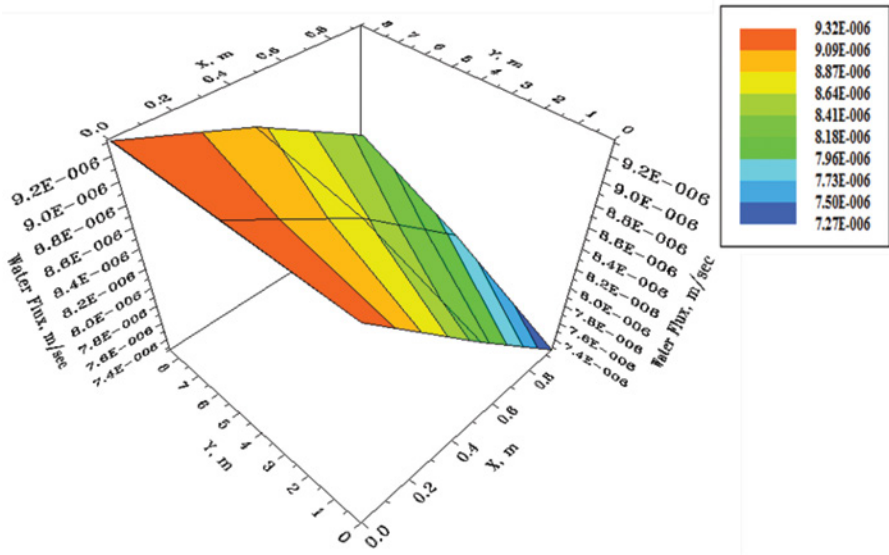


FIGURE 6.44 Water flux in the two dimensions at inlet conditions ($2.583\text{E-}4\text{ m}^3/\text{s}$, $6.548\text{E-}3\text{ kmol}/\text{m}^3$, 13.58 atm , and $31.5\text{ }^\circ\text{C}$).
(Adapted from Al-Obaidi et al., 2017b)

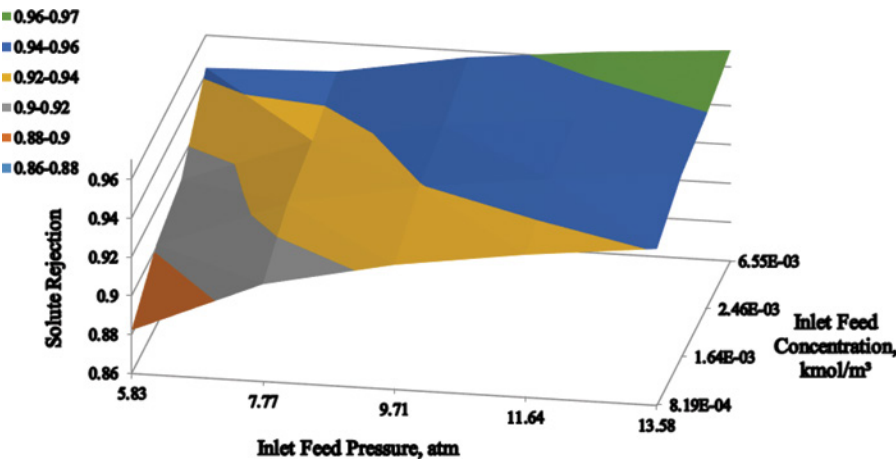


FIGURE 6.45 Impact of variation in inlet feed pressure and concentration on solute rejection at fixed inlet feed flow rate and temperature ($2.583\text{E-}4\text{ m}^3/\text{s}$ and $31\text{ }^\circ\text{C}$).
(Adapted from Al-Obaidi et al., 2017b)

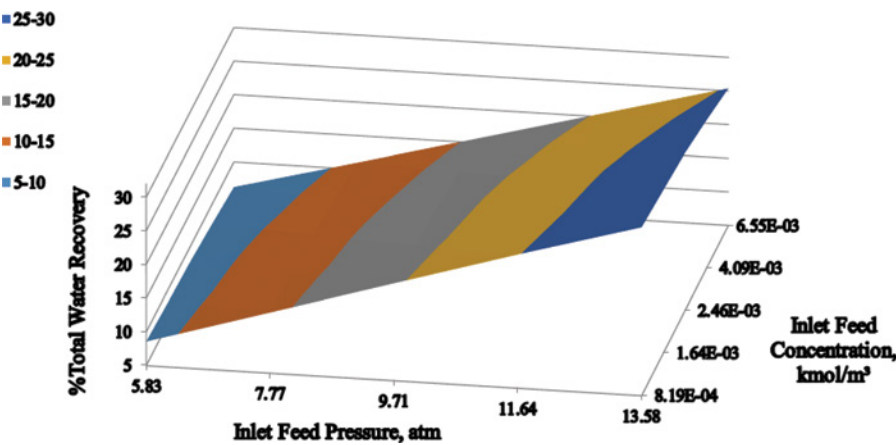


FIGURE 6.46 Impact of variation in inlet feed pressure and concentration on %total water recovery at fixed inlet feed flow rate and temperature ($2.583\text{E-}4\text{ m}^3/\text{s}$ and $31\text{ }^\circ\text{C}$).
(Adapted from Al-Obaidi et al., 2017b)

the operating pressure is increased. However, a decline in the water recovery yields an increasing feed concentration due to the impact of concentration polarisation, which inherently retards the water flux.

The impact of the feed flow rate variation between $2.166\text{E-}4$ and $2.583\text{E-}4\text{ m}^3/\text{s}$ and operating pressure between 5.83 and 13.58 atm at fixed feed concentration and temperature of $6.548\text{E-}3\text{ kmol/m}^3$ and $31\text{ }^\circ\text{C}$, respectively, is depicted in Figure 6.47. Note that $6.548\text{E-}3\text{ kmol/m}^3$ is the maximum operating concentration used in the experiments of Srinivasan et al. (2011). Interestingly, Figure 6.47 shows a different impact of the increasing feed flow rate at high feed concentration and pressure conditions on the dimethylphenol rejection compared to when deploying high feed concentration and low pressure conditions.

At high operating pressures, it is expected that the water flux will be increased due to a decrease in the osmotic pressure. However, increasing the operating pressure corresponds to an increasing level of friction, and at the same time, a high possibility of concentration polarisation at high feed concentration, which ultimately reduces the driving force ($\Delta P_b - \Delta \pi$) of the water flux. It can therefore be said that at such conditions, there is somehow a conflict between the operating variables themselves, which may explain the poor response of the solute rejection at high operating pressures. On the other hand, at low operating pressure conditions, increasing the inlet feed flow rate would significantly reduce the concentration polarisation and solute flux through the membrane. This positively affects the dimethylphenol rejection due to the reduction of the dimethylphenol concentration at the permeate channel.

Furthermore, the implementation of low feed concentration conditions confirms a direct increase in the dimethylphenol rejection as a result of increasing the inlet feed flow rate. This may be caused by a lack of concentration polarisation, which causes an increase in the dimethylphenol rejection as given in Tables 5.14 to 5.16 (Chapter 5).

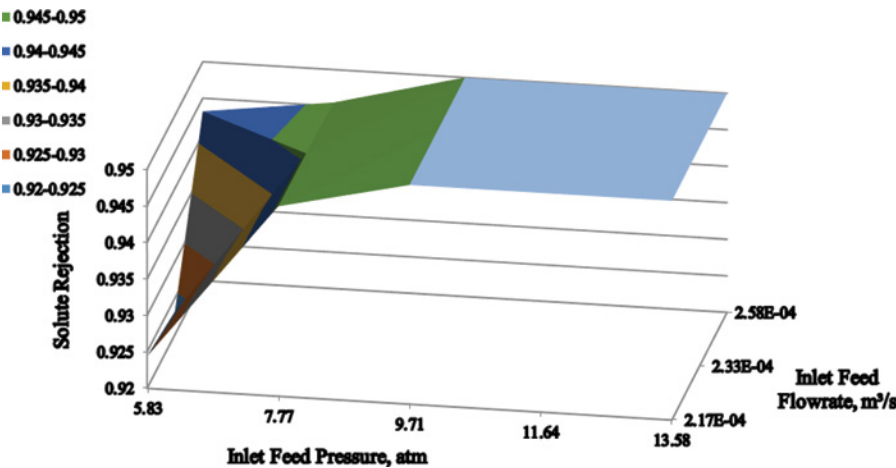


FIGURE 6.47 Impact of variation in inlet feed pressure and flow rate on solute rejection at fixed inlet feed concentration and temperature ($6.548\text{E-}3\text{ kmol/m}^3$ and $31\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi et al., 2017b)

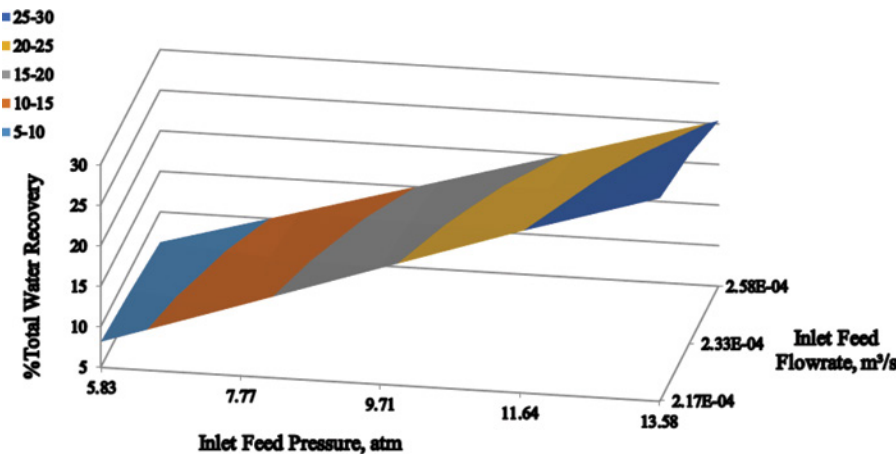


FIGURE 6.48 Model simulation of total water recovery at varying inlet feed flow rates and inlet feed pressures at fixed inlet feed concentration temperature ($6.548\text{E-}3\text{ kmol/m}^3$ and $31\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi et al., 2017b)

The impact of the feed flow rate variation on the total water recovery is shown in Figures 6.48 and 6.49. These figures show a decline in water recovery due to increasing feed flow rate in spite of the reduced osmotic pressure. This can be attributed to the increased frictional pressure drop along the membrane length as a result of the increased feed flow rate. This reduces the driving force of water flux and the

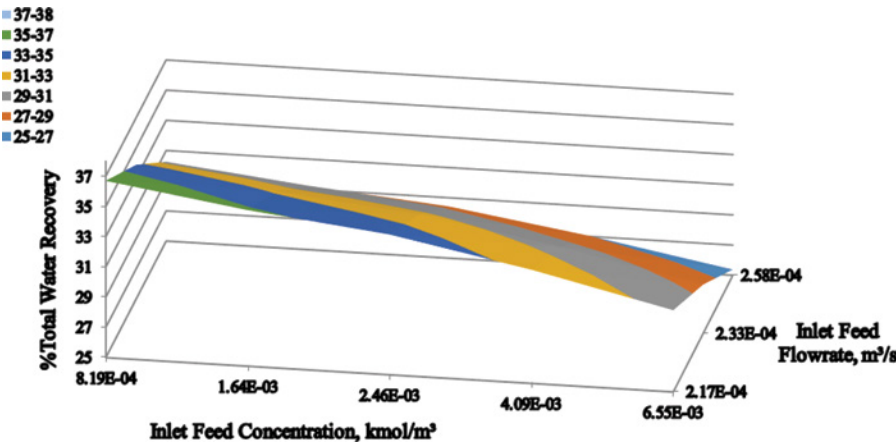


FIGURE 6.49 Impact of variation in inlet feed concentration and flow rate on total water recovery at fixed inlet feed pressure and temperature (13.58 atm and 31 °C).
(Adapted from Al-Obaidi et al., 2017b)

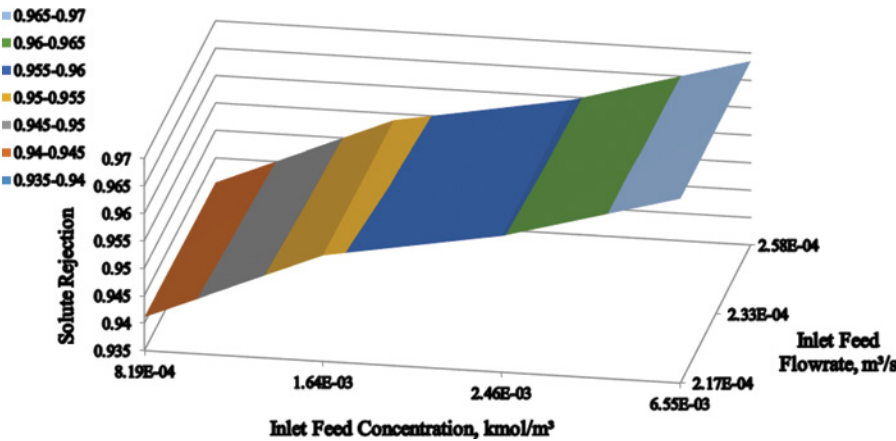


FIGURE 6.50 Impact of variation in inlet feed concentration and flow rate on solute rejection at fixed inlet feed pressure and temperature (13.58 atm and 31 °C).
(Adapted from Al-Obaidi et al., 2017b)

residence time of the bulk feed inside the module. On the other hand, increasing the operating concentration increases the recovery rate due to the reduction in water flux (Figure 6.49).

To precisely understand the response of the dimethylphenol rejection in terms of the variation of the feed concentration, Figure 6.50 presents the variation of the feed concentration and the inlet feed flow rate between 0.819E-3 and 6.548E-3 kmol/m³,

and $2.166\text{E-}4$ and $2.583\text{E-}4$ m^3/s , respectively, at the fixed feed pressure and temperature of 13.58 atm and 31°C , respectively. It is important to note that this simulation is carried out at the highest operating pressure used in the experimental work of Srinivasan et al. (2011). In this respect, a weighty impact of feed concentration change on the dimethylphenol rejection at high operating pressure is clearly observed compared to a feed flow rate change (Figure 6.50).

6.4.10 REMOVAL OF PHENOL FROM WASTEWATER IN AN INDIVIDUAL SPIRAL WOUND RO PROCESS

The removal of phenol and phenolic compounds from industrial wastewater is a critical environmental challenge due to their harmful threats to humans and wild-life. Model XIV (Chapter 5, Al-Obaidi et al., 2017c) and the experimental results of Srinivasan et al. (2010) have been used to investigate in detail the performance of a spiral wound RO process for the removal of phenol from wastewater.

6.4.10.1 Sensitivity Analysis

The parameters studied by Al-Obaidi et al. (2017c) include the operating pressure, concentration, and feed flow rate.

Figure 6.51 shows the impact of the feed pressure on the total permeate flow rate of phenol solutions for two different inlet feed concentrations.

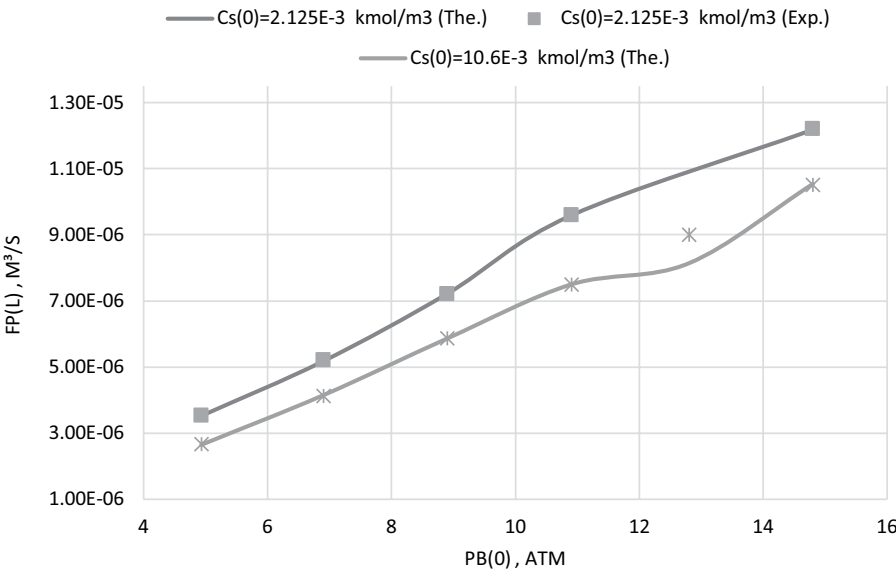


FIGURE 6.51 Experimental and model prediction of total permeated flow rate versus inlet feed pressure for two different inlet feed concentrations at ($F_{b(0)} = 3.333\text{E-}4 \text{ m}^3/\text{s}$ and 33°C). (Adapted from Al-Obaidi et al., 2017c)

A linear positive relationship between the operating pressure and total permeate flow rate at fixed feed flow rate and temperature can be seen in Figure 6.52. However, any increase of the operating concentration reduces the total permeate flow rate (Figure 6.52) due to the increasing osmotic pressure that retards the driving force of water flux.

The impact of operating pressure on phenol rejection at a fixed feed flow rate and temperature is shown in Figure 6.52 for feed solutions of two different concentrations. Here again, the applied pressure has a positive impact on the phenol rejection regardless of the feed concentration used. This is due to a higher resulting water flux caused by an increasing feed pressure, which in turn helps to reduce the phenol concentration at the permeate channel. However, the simulation results of Figure 6.52 confirm that a higher feed concentration yields a higher phenol rejection, as more particularly explained in the next section.

Al-Obaidi and Mujtaba (2016) arrived at similar conclusions when they attempted to remove chlorophenol from wastewater. They observed an increasing solute rejection intensity of the membrane due to the increasing feed concentration. Increasing the latter significantly increases the phenol concentration at the feed channel despite an insignificant increase of phenol concentration at the permeate channel. This particular trend is observed in all the three types of membranes tested by Gómez et al. (2009). It is worth noting here that the model developed by Al-Obaidi et al. (2017c) is in good agreement with the experimental data used for the prediction of phenol rejection, as shown in Figure 6.52.

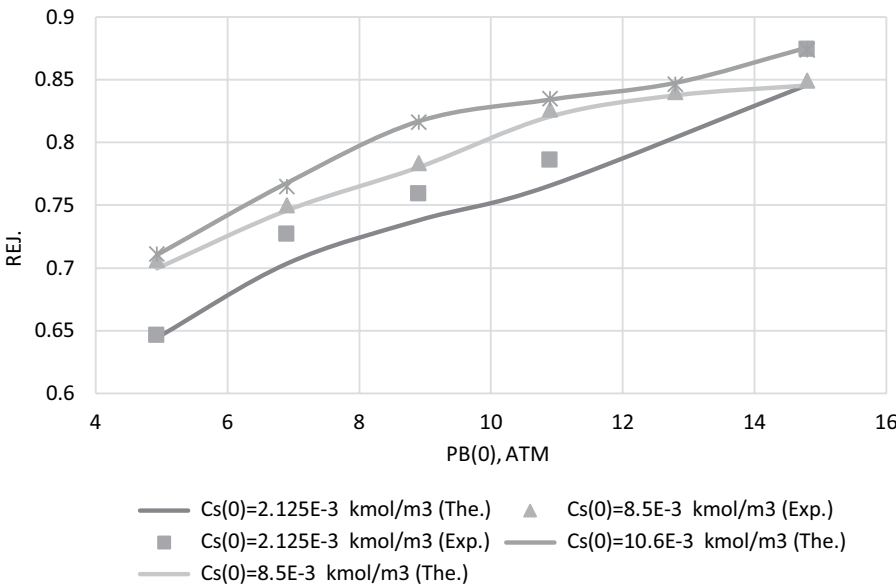


FIGURE 6.52 Experimental and model prediction of phenol rejection versus inlet feed pressure of different inlet feed concentrations at ($F_{b(0)} = 3.33E-4 \text{ m}^3/\text{s}$ and $33 \text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi et al., 2017c)

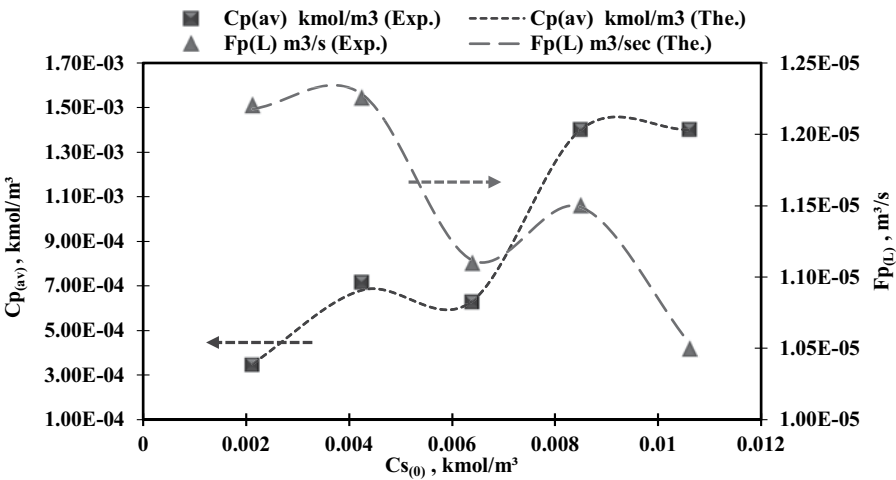


FIGURE 6.53 Experimental and model predictions of phenol permeated concentration and outlet permeated flow rate versus inlet feed concentration (inlet feed conditions, 14.8 atm and 3.33E-4 m³/s, and 33 °C).
(Adapted from Al-Obaidi et al., 2017c)

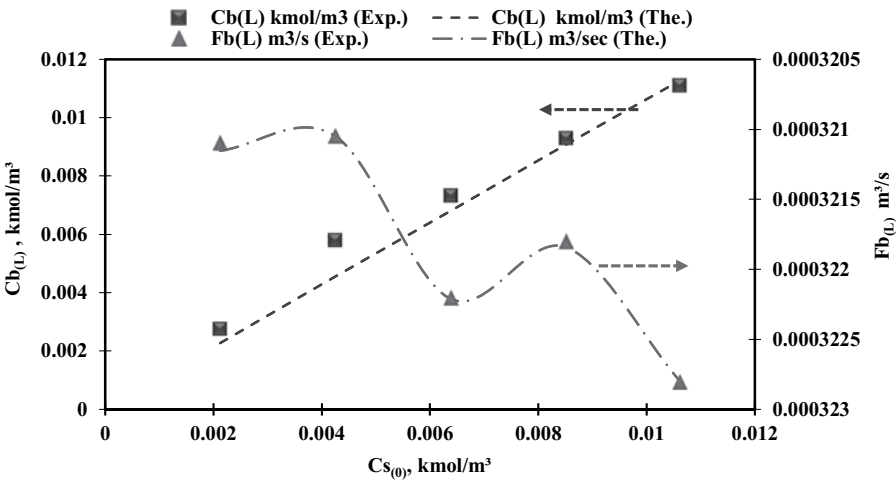


FIGURE 6.54 Experimental and model predictions of retentate phenol concentration and retentate flow rate versus inlet feed concentration (inlet feed conditions, 14.8 atm and 3.33E-4 m³/s, and 33 °C).
(Adapted from Al-Obaidi et al., 2017c)

Figure 6.53 shows the impact of increasing the feed concentration on the permeate concentration and the total permeate flow rate at fixed feed flow rate, pressure, and temperature. Figure 6.53 clearly shows an increase in the average permeate concentration of phenol and a decrease in the total permeate flow rate due to an increasing feed concentration. Basically, increasing the bulk concentration at the feed channel reduces the water flux and consequently reduces the total permeate flow rate, which elevates the phenol concentration at the permeate channel. Indeed, increasing the feed concentration actually increases the retentate concentration of phenol as shown in Figure 6.54. This also increases the retentate flow rate due to the retardation of water flux when increasing the feed concentration.

Figure 6.55 shows that an increase of the inlet feed concentration up to $4.25\text{E-}3\text{ kmol/m}^3$ causes a reduction of phenol rejection at the high operating pressure conditions of 14.8 atm. This is caused by an increase of the osmotic pressure caused by increasing the operating concentration, which reduces the phenol rejection. However, a clear increase of phenol rejection is noticed after applying higher feed concentrations of $8.5\text{E-}3$ to $10.6\text{E-}3\text{ kmol/m}^3$. It seems that increasing the feed concentration up to these conditions would increase the membrane rejection intensity, which aids in attaining a higher phenol rejection rate. Simulation results of this same case study have been used to investigate the optimum feed concentration of $6.375\text{E-}3\text{ kmol/m}^3$, which yields a maximum phenol rejection (Figures 6.55 and 6.56).

Figure 6.56 clearly shows that increasing the feed concentration at an average operating pressure of 8.9 atm has the same positive impact on the phenol rejection except for the case of $6.375\text{E-}3\text{ kmol/m}^3$ of feed concentration. These results are in good agreement with the findings of Srinivasan et al. (2011) and Sundaramoorthy et al. (2011) for both dimethylphenol and chlorophenol rejection, respectively.

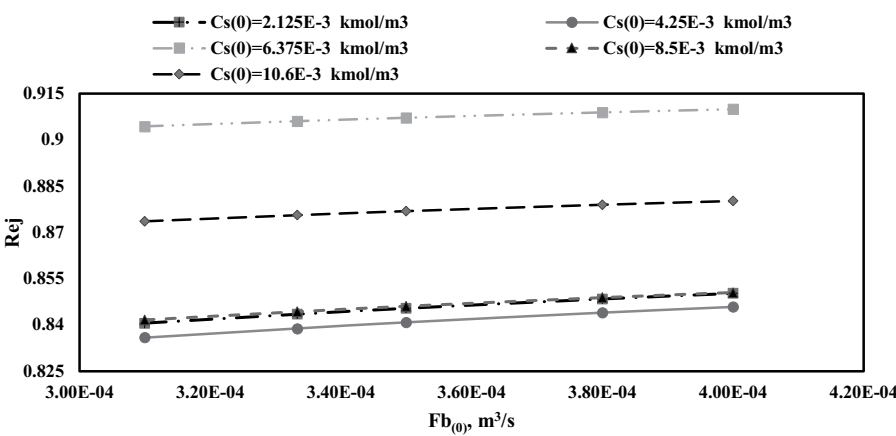


FIGURE 6.55 Phenol rejection versus inlet feed flow rate for different inlet feed concentrations (inlet feed conditions, 14.8 atm, and 33 °C).

(Adapted from Al-Obaidi et al., 2017c)

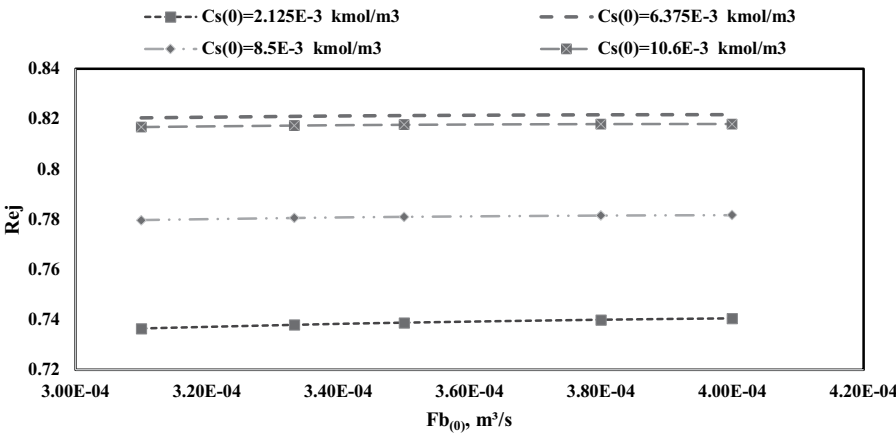


FIGURE 6.56 Phenol rejection versus inlet feed flow rate for different inlet feed concentrations (inlet feed conditions, 8.9 atm, and 33 °C).

(Adapted from Al-Obaidi et al., 2017c)

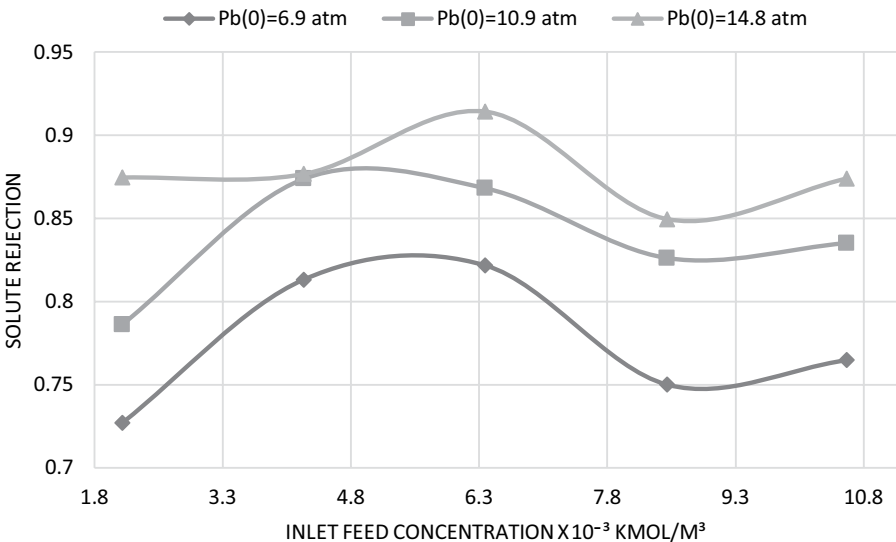


FIGURE 6.57 Solute rejection versus inlet feed concentration for three different inlet feed pressures (inlet feed conditions 3.333×10^{-4} m³/s and 32.2–34.5 °C).

(Adapted from Al-Obaidi et al., 2017d)

Another conclusion which can be made from Figures 6.55 and 6.56 is that the inlet feed flow rate at high operating pressure has a noticeable impact on the phenol rejection compared to that at middle operating pressure.

Al-Obaidi et al. (2017d) used another one-dimensional model (Model XIII described in Chapter 5), which was developed to investigate the removal of phenol,

using the same membrane type of the previous study. They studied the impact of inlet feed concentration on the phenol rejection for low, middle, and high operating pressures. These same operating conditions were used by Srinivasan et al. (2010) in their experiments of phenol removal from wastewater. Figure 6.57 shows that increasing the operating pressure causes an increase in the phenol rejection due to an increase of water permeation through the membrane for all the feed concentrations tested. The simulation results of Figure 6.57 indicate the same observations derived from Figures 6.55 and 6.56, where a maximum phenol rejection is observed at an operating concentration close to $6.375\text{E-}3 \text{ kmol/m}^3$. This same figure also shows the progress of phenol rejection at lower feed concentration conditions due to increasing the inlet feed concentration. The phenol rejection reduces at higher feed concentrations due to a higher osmotic pressure, which causes a decrease in the driving force of water flux.

6.4.11 REMOVAL OF DIMETHYLPHENOL FROM WASTEWATER IN A MULTI-STAGE RO PROCESS

Al-Obaidi et al. (2018a) explored the impact of network configuration of three spiral wound RO membranes for the removal of dimethylphenol from wastewater at different feed concentrations using Model X described in Chapter 5 (Al-Obaidi et al., 2017a).

6.4.11.1 Description of Multi-Stage RO Configurations

Al-Obaidi et al. (2018a) proposed several multi-stage RO process configurations for the removal of dimethylphenol from wastewater by considering only three modules connected differently to form four possible RO networks. The main aim of this study was to explore the best configuration that performs the highest dimethylphenol rejection. The system comprises two pressure vessels connected in parallel, and each pressure vessel holds only one spiral wound RO membrane type HM4040-LPE supplied by Ion Exchange (Mumbai, India) with an effective membrane area of 7.85 m^2 . The schematic diagram of the four proposed configurations is given in Figure 6.58. Such configurations are similar to those used by Abbas (2005) for an RO seawater desalination process.

The simple design of the proposed layouts is based on retentate reprocessing, where the concentrated stream of the first membrane element becomes the feed stream of the subsequent element, and so on. In this respect, the permeate streams of three elements are combined to form the product stream of the final layout. For instance, configuration A includes two parallel modules in the first stage, where the feed stream is equally split into two parallel modules, and the concentrate streams of these modules are combined to form the feed stream of the second-stage module. The maximum allowed pressure drop along the membrane length was 1.3817 atm , as recommended by the manufacturer.

6.4.11.2 RO Network Performance Analysis

The performance of the proposed configurations shown in Figure 6.58 was tested for a set of inlet feed concentrations of 1.637 , 2.455 , and 6.548 kmol/m^3 and fixed operating

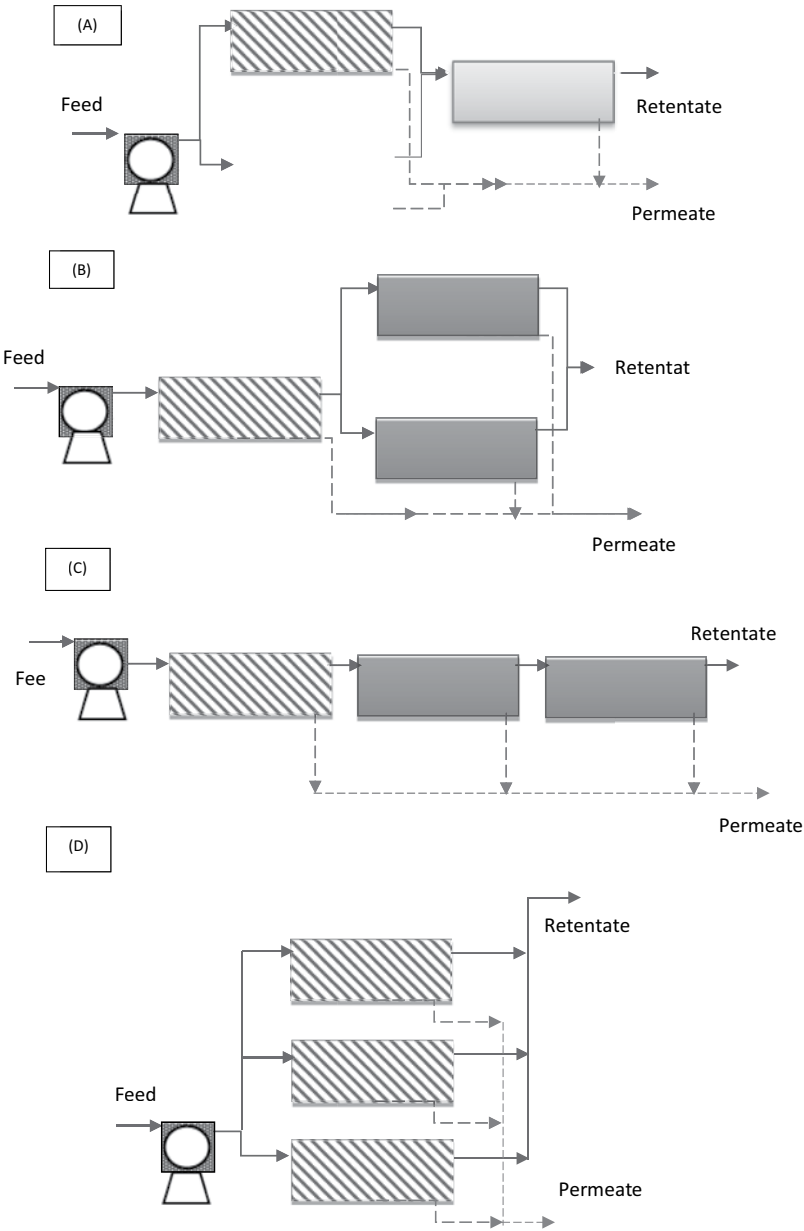


FIGURE 6.58 Schematics of different RO configurations.

(Adapted with permission from Al-Obaidi et al., 2018a)

conditions of inlet flow rate, pressure, and temperature of $4.5\text{E-}4\text{ m}^3/\text{s}$, 16 atm, and $37\text{ }^{\circ}\text{C}$, respectively. The inlet feed flow rate selected for each element are as recommended by the manufacturer. Table 6.1 shows the simulation results of four configurations, which include dimethylphenol rejection and water recovery. Also, the total pressure loss for each configuration selected is included to achieve the cheapest solution.

Table 6.1 confirms that configuration D of a single stage of three parallel modules yielded the highest dimethylphenol rejection and water recovery at the lowest pressure loss compared to the other configurations. However, all the configurations tested achieved relatively high dimethylphenol rejection values at different inlet feed concentrations. It can therefore be said that the parallel configuration is the more affordable solution due to the smallest pressure decrease along the membrane length, which was the result of implementing the same operating conditions tested for all the configurations. Note that the parallel configuration has another immediate advantage of the possibility of increasing the total water recovery in case of using the retentate concentrated stream in a subsequent module due to its high pressure. On the other hand, Table 6.1 shows that the tapered configurations A and B were relatively similar in their dimethylphenol rejection performance, and with a clear difference in their water recovery rate. It is easy to notice the difference in the total water recovery achieved for the four configurations tested. Configurations A and D attained the highest water recovery under the same operating conditions compared to configurations B and C. More specifically, the parallel configuration layout D achieved the highest water recovery due to the lower pressure loss along the membrane feed channel. However, the series configuration C achieved the worst water recovery due

TABLE 6.1
Simulation Results of Four RO Networks

Feed concentration $\times 10^3$, kmol/m ³	Scenario	Dimethylphenol rejection % (–)	Water recovery % (–)	Total configuration pressure loss (atm)
1.637	A	97.76	64.74	3.28
	B	97.70	55.24	4.71
	C	97.76	49.43	8.49
	D	97.72	66.52	0.87
2.455	A	98.04	63.30	3.34
	B	97.96	53.99	4.74
	C	98.00	48.35	8.55
	D	98.01	64.76	0.88
6.548	A	98.51	57.98	3.54
	B	98.42	49.33	4.82
	C	98.41	44.15	8.79
	D	98.50	58.73	0.92

Note: Operating conditions: $6.548\text{E-}3\text{ kmol/m}^3$, $4.5\text{E-}4\text{ m}^3/\text{s}$, 16 atm, and $37\text{ }^{\circ}\text{C}$.
(Adapted with permission from Al-Obaidi et al., 2018a)

to the maximum pressure drop. This is due to the increasing osmotic pressure in the subsequent modules despite having a high feed flow rate. Abbas (2005) confirmed the same results.

The inlet feed concentration has a similar impact on the performance of the RO network in all the four configurations studied (Table 6.1). The reduction of water recovery, besides the increase of dimethylphenol rejection, is achieved when increasing the feed concentration. An increase in the osmotic pressure because of increasing the feed concentration may explain the underlying reason for this, in that it reduces the driving force of the water flux besides increasing the membrane solute isolation intensity, in turn due to an increase in the bulk concentration at the feed channel. The impact of the inlet feed concentration on the retentate flow rate and the total pressure loss of configuration A at fixed inlet feed flow rate, pressure, and temperature is illustrated in Figure 6.59. Clearly, increasing the inlet feed concentration of configuration A results in an increase of the pressure drop due to an increase in the osmotic pressure at the feed channel. This basically reduces the water flux through the membrane pores and therefore increases the bulk feed velocity and retentate flow rate, that in turn results in a higher pressure drop due to the increased friction.

The impact of increasing feed pressure on the total pressure drop and total permeated flow rate for configuration B is illustrated in Figure 6.60. The increase is carried out at fixed feed flow rate, concentration, and temperature. A reduction of the total pressure loss as a result of increasing the operating pressure at a fixed feed flow rate can be observed. Increasing the pressure causes an increase in the water flux penetrating through the membrane, which in turn causes a reduction of the bulk feed flow rate and consequently the retentate flow rate. It is therefore fair to expect a pressure loss reduction.

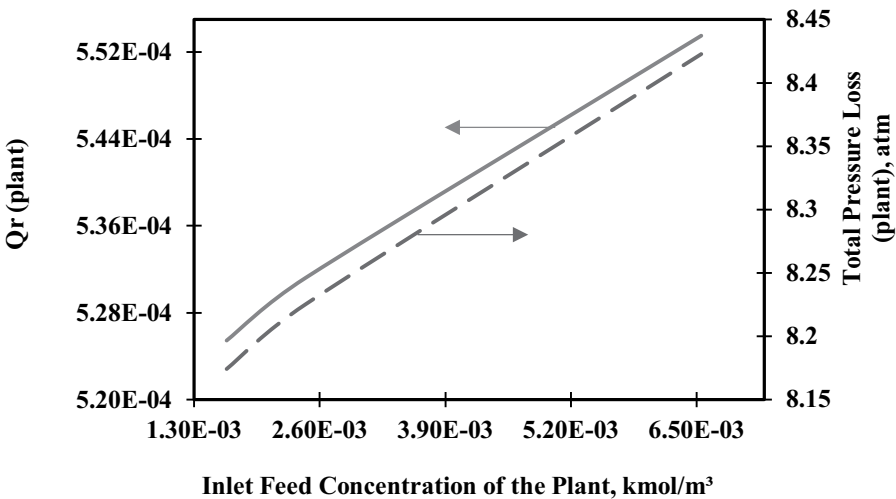


FIGURE 6.59 Inlet feed concentration of the plant as a function of the total pressure loss and retentate rate for configuration A at initial conditions of 8.5112E-4 m³/s, 19 atm, and 35 °C.

(Adapted with permission from Al-Obaidi et al., 2018a)

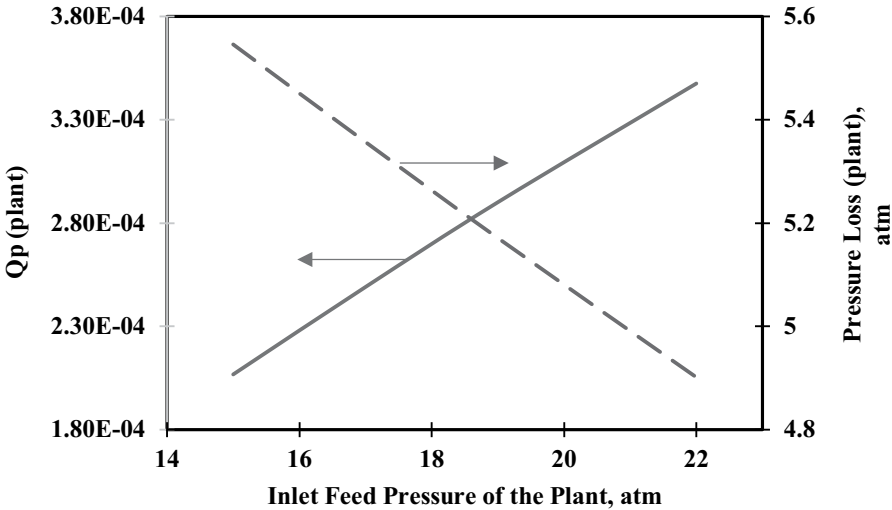


FIGURE 6.60 Inlet feed pressure of the plant as a function to the total pressure loss and permeate flow rate for configuration B at initial conditions of 5E-4 m³/s, 2.455E-3 kmol/m³, and 34 °C.

(Adapted with permission from Al-Obaidi et al., 2018a)

Figure 6.61 shows the impact of the operating temperature for configuration C on the dimethylphenol rejection and the total pressure loss at a fixed feed concentration, flow rate, and pressure. A significant positive impact of temperature on the dimethylphenol rejection is observed as a result of increasing the water flux. Also, a reduction in pressure loss is noticed when increasing the temperature, due to a reduction in the bulk velocity inside the feed channel.

The impact of feed flow rate on the total recovery rate and pressure loss of configuration D is illustrated in Figure 6.62 at fixed feed concentration, pressure, and temperature. Increasing the feed flow rate causes a reduction in the total water recovery due to the reduction in the residence time of the bulk fluid inside the feed channel. This reduces the total water flux and in turn increases the total pressure loss.

Figure 6.63 shows the impact of the inlet feed flow rate on the dimethylphenol rejection and the total water recovery of all the configurations tested as shown in Figure 6.58, considering the operating conditions of 6.548 kmol/m³, 17.7 atm, and 32 °C, of feed concentration, pressure, and temperature, respectively. Increasing the feed flow rate causes an increase in the dimethylphenol rejection for all the previously listed configurations. The reduction occurring in the concentration polarisation as a result of increasing the feed velocity can explain the reason for this. Having said this, the total water recovery decreases when increasing the feed flow rate. This is because of the reduced residence time of the bulk fluid inside the feed channel, which retards the water flux through the membrane. It can therefore be said that any RO network with a lower feed flow rate along its modules will enhance the possibility of gaining a higher water recovery because of the reduced pressure drop along

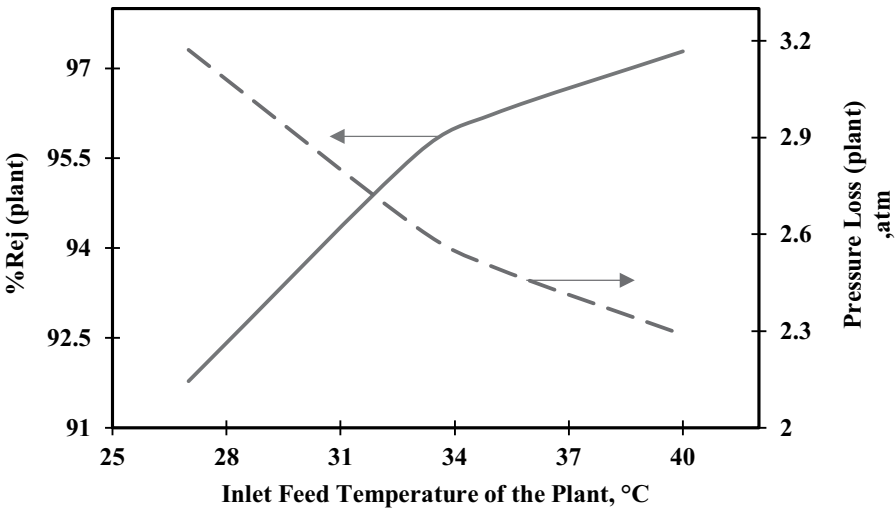


FIGURE 6.61 Inlet feed temperature of the plant as a function of the total pressure loss and rejection for configuration C, at initial conditions of $2\text{E-}4\text{ m}^3/\text{s}$, $6.548\text{E-}3\text{ kmol}/\text{m}^3$, and 15 atm.

(Adapted with permission from Al-Obaidi et al., 2018a)

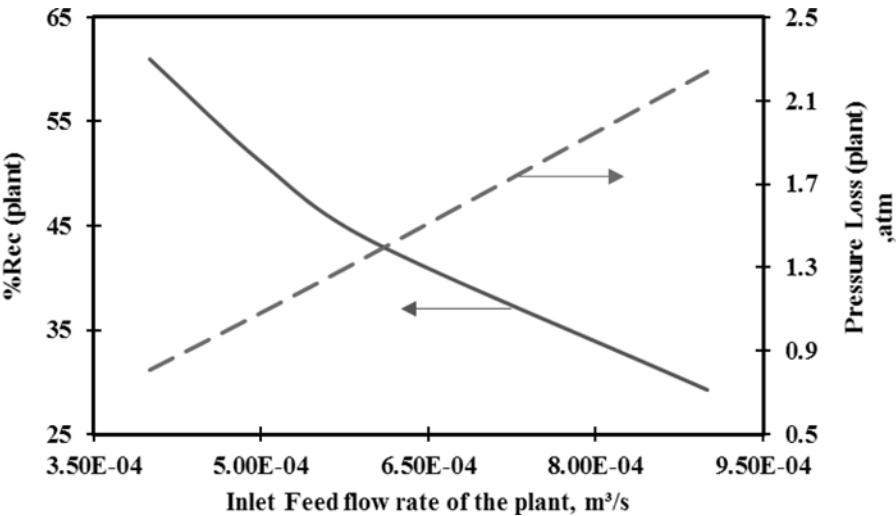


FIGURE 6.62 Inlet feed flow rate of the plant as a function of the total pressure loss and recovery for configuration D at initial conditions of $6.548\text{E-}3\text{ kmol}/\text{m}^3$, 15.5 atm, and 36 °C.

(Adapted with permission from Al-Obaidi et al., 2018a)

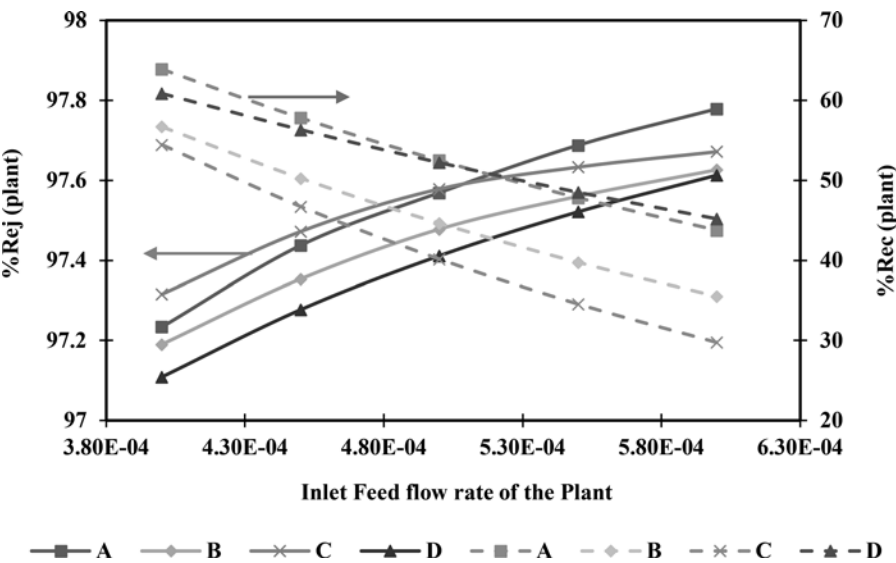


FIGURE 6.63 Inlet feed flow rate of the plant as a function of the rejection and recovery rate for four RO configurations (A, B, C, and D).

(Adapted with permission from Al-Obaidi et al., 2018a)

the membrane length. Figure 6.63 shows that configuration D offers a higher water recovery with a high rejection compared to other layouts at the same operating conditions, due to attaining the lowest pressure drop.

6.4.12 REMOVAL OF NITROSAMINE FROM WASTEWATER IN A LOW-PRESSURE RO PROCESS

Fujioka et al. (2012) used a bench-scale crossflow filtration system of low-pressure RO process, using a membrane type TFC-HR with an effective membrane area of 40 cm², to study the capacity of removing eight N-nitrosamine compounds from the synthesised wastewater of 250 ng/L of each N-nitrosamine compound, including NDMA. Figure 6.64 illustrates the schematic diagram of the RO process. A sensitivity analysis was then carried out using the irreversible thermodynamic model developed by Kedem and Katchalsky (1963) to assess the process performance under varying operating conditions.

6.4.12.1 Sensitivity Analysis of Operating Conditions

Increasing the operating pressure at fixed operating feed velocity, solution pH, and temperature increase the permeate flux through the membrane, which in turn increases the N-nitrosamine rejection as depicted in Figure 6.65. The variation of permeate flux from 5 to 60 L/m² h causes an improvement of NDMA rejection from 25% to 63%. (However, the rejection of NDBA increases from 49% to 89%.) The improvements of NDMA and NMEA rejections (two smallest N-nitrosamines) are

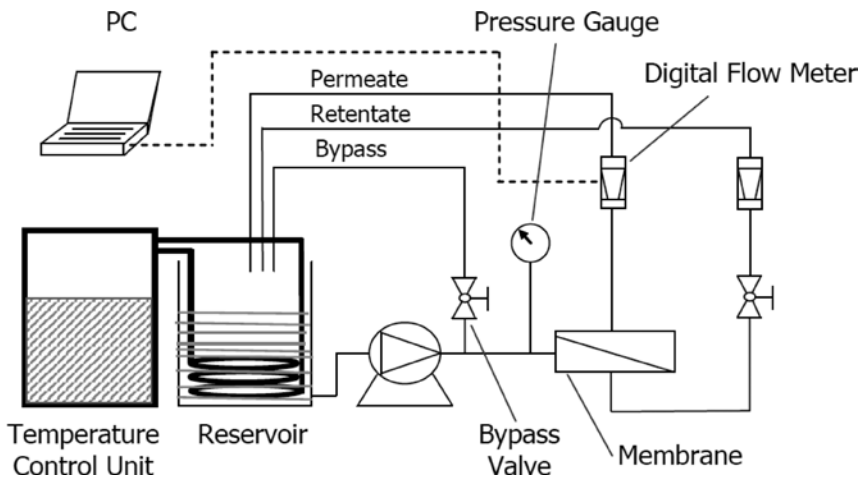


FIGURE 6.64 Schematic diagram of the crossflow RO filtration system.

(Adapted from Fujioka et al., 2012)

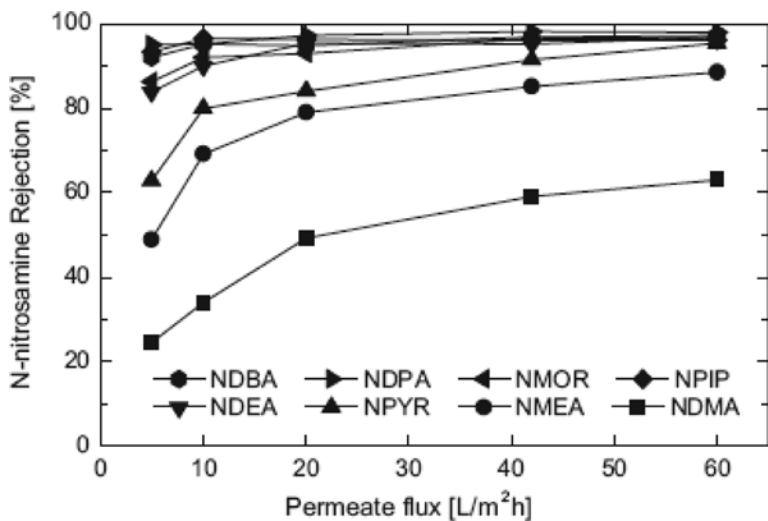


FIGURE 6.65 N-nitrosamine rejection against permeate flow at different operating pressures (operating conditions: crossflow velocity 40.2 cm/s, feed pH 8.0 ± 0.1, and temperature 20.0 ± 0.1 °C).

(Adapted from Fujioka et al., 2012)

found to be in the range of permeate flux of less than 20 L/m² h. The low rejection of NDMA and NMEA can be attributed to their high hydrophilicity and it is therefore fair to expect a low possibility of these being adsorbed at the membrane surface.

The variation of feed concentration from 250 ng/L to 1500 ng/L at fixed feed velocity, permeate flux, solution pH, and temperature was applied to investigate the

performance of the process of removing N-nitrosamine. Figure 6.66 shows an insignificant increase of N-nitrosamine rejection for the variation tested. This might be attributed to the limitation of the irreversible thermodynamic model to accurately determine the rejection parameter when varying the feed concentration. In other words, this model considered the solute rejection as an independent variable of the feed solute concentration.

The influence of the operating temperature from 10 to 40 °C at fixed feed velocity, permeate flux, and pH on N-nitrosamine rejection is shown in Figure 6.67. A reduction of all the N-nitrosamine rejections tested as a response to increasing the operating temperature is observed. This can be attributed to the increasing pore size of the membrane and the solute flux as a response to the temperature increase. Sharma et al. (2003) observed the same in their studies.

The impact of increasing the feed solution pH from 3.5 to 9 on the N-nitrosamine rejection was investigated at constant feed velocity, permeate flux, and temperature. Figure 6.68 presents the progress of N-nitrosamine rejection as a result of increasing the pH solution. This can be attributed to decreasing the pore size in addition to the change of membrane polymeric matrix as a response to increasing the pH. The rejection of NDMA, NMEA, and NPYR dropped from 49% to 24%, 81% to 62%, and 90% to 74%, as a result of decreasing solution pH from 9 to 3.5, respectively. Similar observations were reported by Childress and Elimelech (2000).

Steinle-Darling et al. (2007) used a bench-scale crossflow filtration RO system, which contains a flat sheet membrane (103 cm²) type ESPA3 (Hydramautics, Oceanside, CA, USA) to treat wastewater containing polar, uncharged seven N-nitrosoalkylamines with molecular masses varying between 78 and 158 Da. The

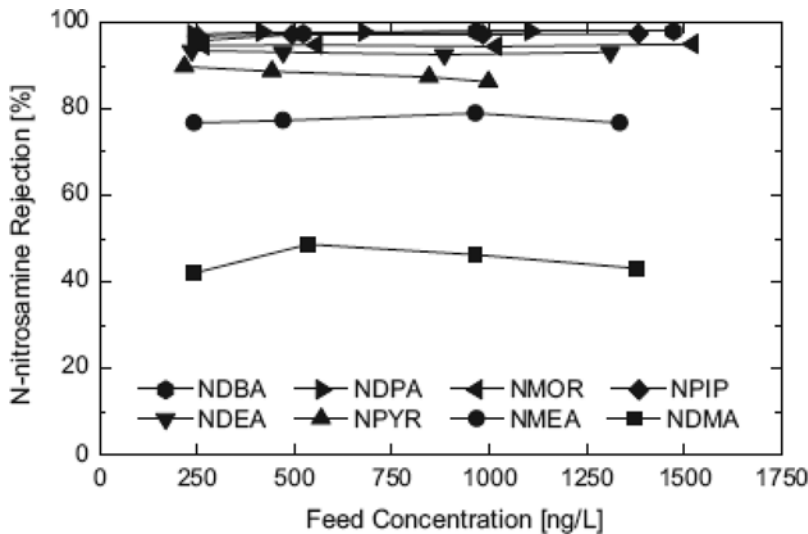


FIGURE 6.66 N-nitrosamine rejection against feed concentration (operating conditions: crossflow velocity 40.2 cm/s, feed pH 8.0 ± 0.1, permeate flux 20 L/m² h, and temperature 20.0 ± 0.1 °C).

(Adapted from Fujioka et al., 2012)

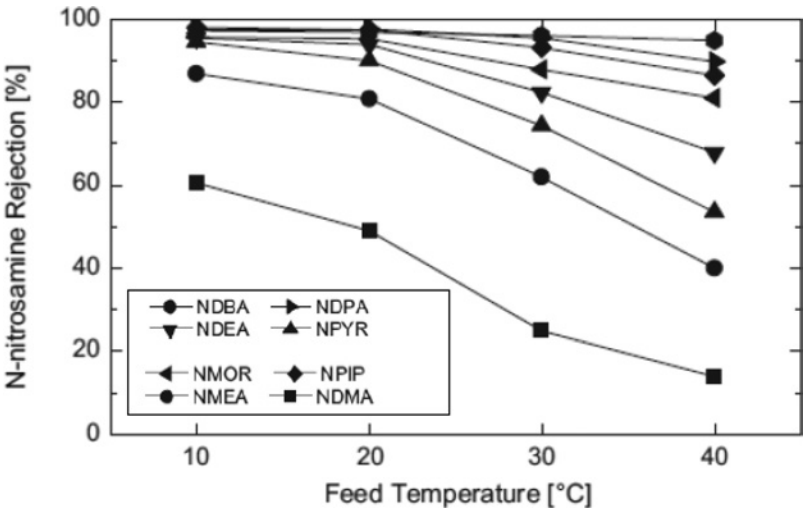


FIGURE 6.67 N-nitrosamine rejection against feed temperature (operating conditions: crossflow velocity 40.2 cm/s, feed pH 8.0 ± 0.1 , and permeate flux 20 L/m² h).
(Adapted from Fujioka et al., 2012)

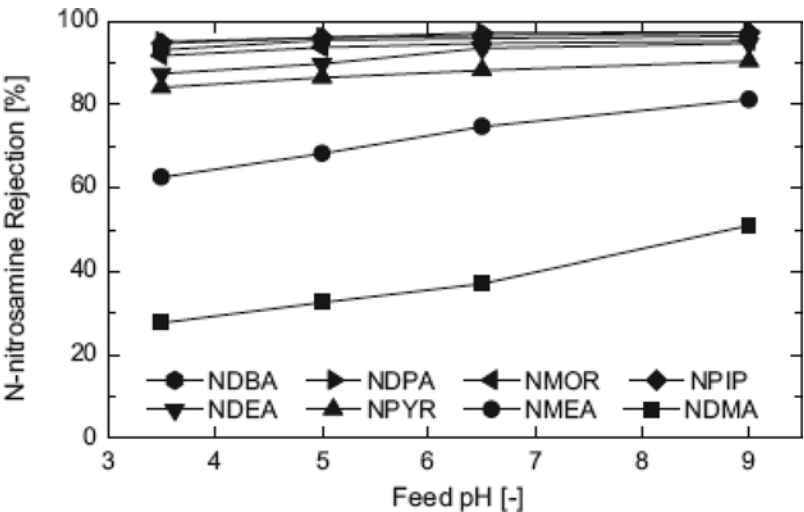


FIGURE 6.68 N-nitrosamine rejection against feed pH (operating conditions: crossflow velocity 40.2 cm/s, permeate flux 20 L/m² h, and temperature 20.0 ± 0.1 °C).
(Adapted from Fujioka et al., 2012)

experimental tests confirmed that decreasing the pH to 3 decreased the rejection rate by 5%. However, increasing the pH to 10 has insignificant impact on the rejection.

6.4.13 REMOVAL OF NITROSAMINE FROM WASTEWATER IN FULL-SCALE MULTI-STAGE RO PROCESS

Al-Obaidi et al. (2017e) simulated the full-scale RO wastewater treatment system of Fujioka et al. (2014) shown in Figure 6.69 using a series of seven 4" glass-fibre pressure vessels (one membrane per each pressure vessel, make: Hydranautics, Oceanside, CA, USA). The simulation was carried out using a one-dimensional steady state model (Model IX, Chapter 5, Al-Obaidi et al., 2017f) developed for a single spiral wound RO process. The model was calibrated to satisfy the estimation of NDMA removal using the multi-stage RO process.

Figures 6.70 and 6.71 show the effect of the total NDMA rejection and water recovery against the variation of operating pressure and feed flow rate from 4 to 18 atm and $7.85\text{E-}4$ to $2.5\text{E-}3$ m^3/s at fixed feed concentration and temperature of $250\text{E-}6$ ppm and 20°C , respectively.

A close look at Figure 6.70 confirms the highest NDMA rejection of 52% at the operating conditions of 15.9 atm and $2.5\text{E-}3$ m^3/s of pressure and flow rate, respectively. Any increase of pressure helps the NDMA rejection, especially at low feed flow rates, due to the increasing water flux, which reduces NDMA concentration at the permeate channel. Interestingly, Figure 6.70 shows a slight reduction of NDMA rejection as a result of increasing the operating pressure with a feed flow rate varying from $1.5\text{E-}3$ to $2.5\text{E-}3$ m^3/s . This can be attributed to increasing the bulk concentration and osmotic pressure at the feed side. This is due to the high water flux, which in turn retards the rejection, in turn due to decreasing the water flux through the membrane. This can be clearly seen in Figure 6.71, where a small reduction in water recovery occurs with a feed flow rate varying from $1.5\text{E-}3$ to $2.5\text{E-}3$ m^3/s . The same was not observed for the feed flow rate varying from $7.85\text{E-}4$ to $1.5\text{E-}3$ m^3/s , where any increase of pressure gradually improves the NDMA rejection, with an approximately constant water recovery (Figure 6.71).

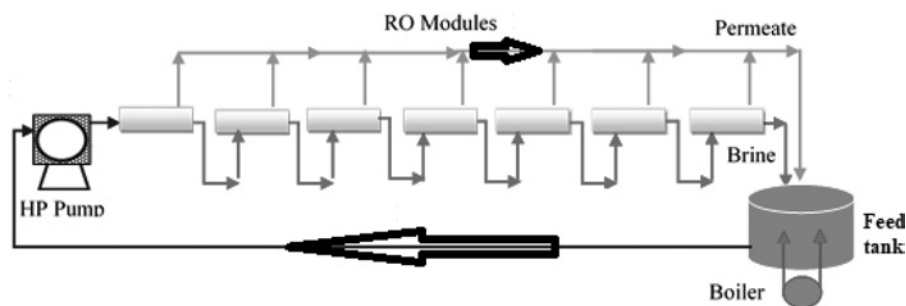


FIGURE 6.69 Schematic diagram of full-scale seven-element RO plant used by Fujioka et al. (2014).

(Adapted from Al-Obaidi et al., 2017e)

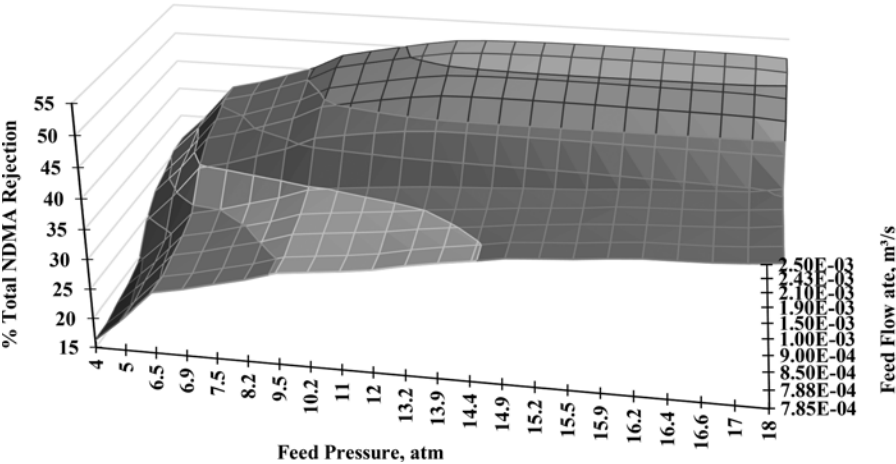


FIGURE 6.70 Impact of variation in feed pressure and flow rate on total NDMA rejection at fixed inlet feed concentration and temperature (250E-6 ppm and 20 °C).

(Adapted from Al-Obaidi et al., 2017e)

Figure 6.70 shows that increasing the feed flow rate causes an increase of the NDMA rejection, which can be attributed to the reduction of the osmotic pressure. Increasing the flow rate at the feed channel causes an increase of the mass transfer coefficient, which mitigates the concentration polarisation and NDMA concentration at the membrane surface. It can therefore be argued that a high feed flow rate is critical for NDMA rejection. The optimum operating conditions of 2.5E-3 m³/s and 15.9 atm corresponding to the maximum NDMA rejection, Figure 6.70, confirm that the corresponding increase of feed flow rate from 7.85E-4 to 2.5E-3 m³/s can enhance the NDMA rejection to around 41%. Also, the increase of operating pressure from 4 to 18 atm can enhance the NDMA rejection to around 67%.

Figure 6.71 shows that running the process at the maximum pressure tested at 18 atm and the lowest feed flow rate of 7.85E-4 m³/s yield a maximum water recovery of around 40%. However, any further increase of feed flow rate would passively impact the water recovery, especially after 1E-3 m³/s. The increase of pressure drop for each element due to increasing the feed flow rate can explain this phenomenon, which retards the driving force of water flux in addition to reducing the residence time of feed inside the modules.

The impact of the feed concentration variation from 74.05E-6 to 370.25E-6 ppm and operating pressure from 4 to 18 atm on the NDMA rejection at a fixed feed flow rate and temperature of 8.5E-4 m³/s and 20 °C (Case 1), respectively, is shown in Figure 6.72. Figure 6.73 shows simulation results for the same operating conditions but at higher and constant feed flow rates of 2.43E-3 m³/s (Case 2).

Figures 6.72 and 6.73 indicate that the maximum NDMA rejection of around 55.1% can be achieved at the maximum tested pressure and concentration of 18 atm and 370.25E-6 ppm, respectively. These results reflect the poor performance of the

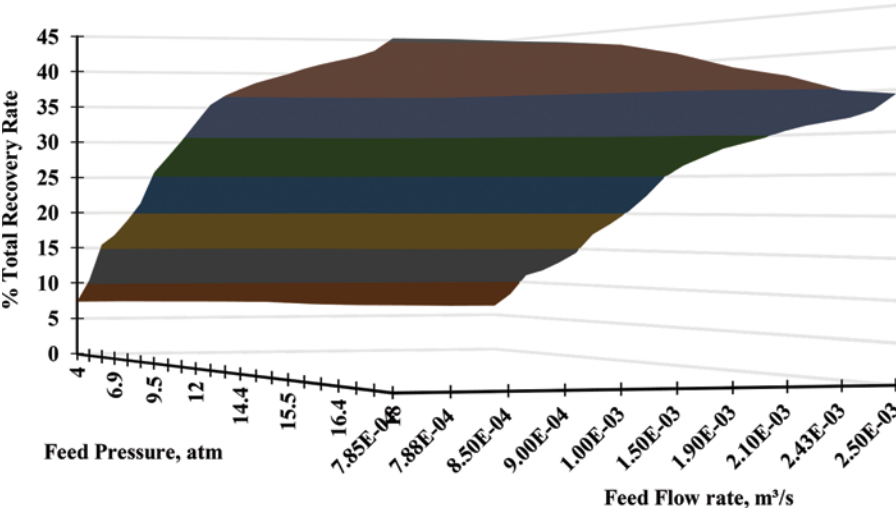


FIGURE 6.71 Impact of variation in feed pressure and flow rate on total recovery rate at fixed inlet feed concentration and temperature (250E-6 ppm and 20 °C).
(Adapted from Al-Obaidi et al., 2017e)

proposed multi-stage series RO configuration for the removal of NDMA from wastewater. This has already been investigated by several researchers, including Steinle-Darling et al. (2007), Plumlee et al. (2008), Krauss et al. (2010), and Fujioka et al. (2014).

Figures 6.72 and 6.73 show that NDMA rejection decreases when the feed concentration for the specific range of low operating pressure increases from 4 to 8.5 atm, as well as for the two cases of low and high feed flow rates of 8.5E-4 and 2.43E-3 m³/s. These figures show that the optimum NDMA rejection appears to start to take place at the specific value of feed concentration of 4 atm. Several studies confirmed the impact of feed concentration on the rejection parameter. For instance, Haluch et al. (2017) affirmed the substantial effect of the feed concentration on solute rejection parameter. They also confirmed an optimal concentration value, which corresponds to an optimum rejection rate for a small-scale desalination unit operating at low pressure and feed flow rate. In summary, it is fair to say that the feed concentration behaves harmoniously against the NDMA rejection for the range of low operating pressures (4 to 8.5 atm) in spite of the operating feed flow rate. The osmotic pressure and concentration polarisation increase as a result of the increasing bulk concentration would explain the reason for this behaviour, in that the water flux and NDMA rejection are decreased immediately. There is an improvement on the other hand, in that the NDMA rejection is enhanced at low concentrations and a low range of operating pressures, more specifically at higher feed flow rate (Figure 6.73). This shows a passive impact of the concentration polarisation, where any reduction of feed concentration helps the mass transfer coefficient and the water flux. Unfortunately, this observation does not hold for feed pressures beyond 8.5 atm, as more specifically indicated in Figures 6.72 and 6.73. A significant increase of NDMA rejection

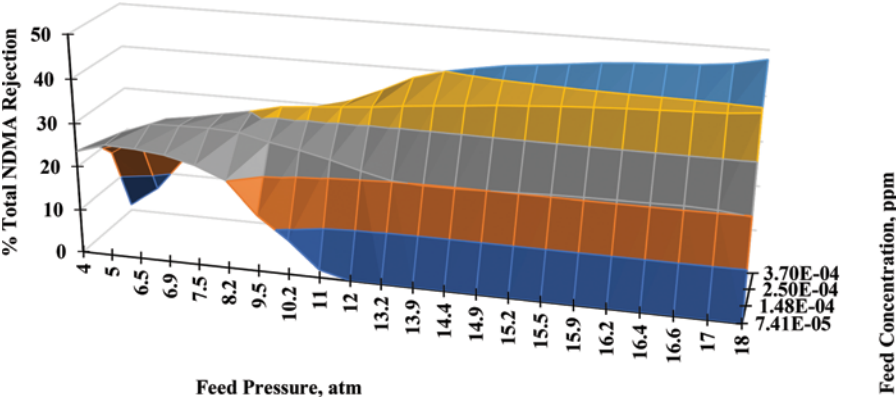


FIGURE 6.72 Impact of variation in feed pressure and concentration (Case 1) on total NDMA rejection at fixed inlet feed flow rate and temperature ($8.5\text{E-}4\text{ m}^3/\text{s}$ and $20\text{ }^\circ\text{C}$). (Adapted from Al-Obaidi et al., 2017e)

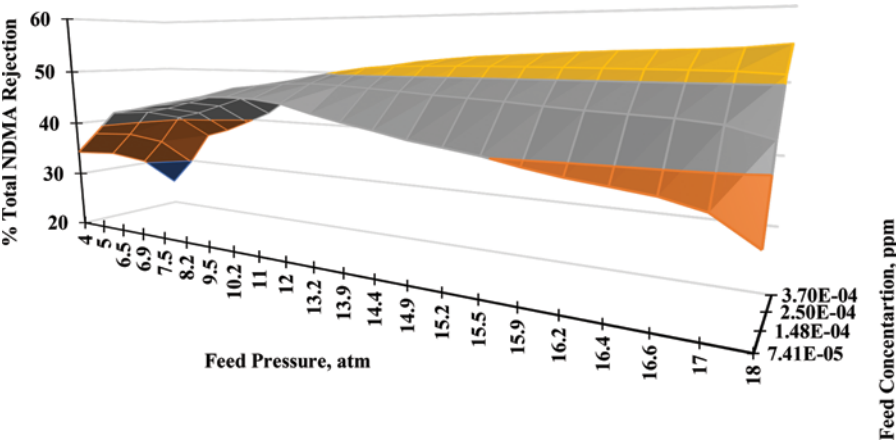


FIGURE 6.73 Impact of variation in feed pressure and concentration (Case 2) on total NDMA rejection at fixed inlet feed flow rate and temperature ($2.43\text{E-}4\text{ m}^3/\text{s}$ and $20\text{ }^\circ\text{C}$). (Adapted from Al-Obaidi et al., 2017e)

is noticed when the feed concentration increased with the feed pressure beyond 8.5 atm. This can be attributed to the increasing water flux that reduces the NDMA concentration at the permeate channel. The latter occurs as a result of working at high operating pressure. It can therefore be said that the NDMA rejection is improved when the feed concentration is increased in the range of high feed pressure up to 8.5 atm. This is caused by the increasing membrane solute rejection intensity due to the increasing bulk concentration (Al-Obaidi and Mujtaba, 2016). Another possible reason for this behaviour is that a feed concentration increase would in fact increase the

bulk concentration, in the same manner as the low NDMA concentration at the permeate channel. In summary, the increase of NDMA rejection is due to the increase in the feed concentration. This statement is agreement with the findings of Gómez et al. (2009).

Figure 6.72 shows zero NDMA rejection for the operating condition of low feed concentration of $74.1\text{E-}6$ ppm, high operating pressures, and low operating feed flow rate of $8.5\text{E-}4$ m³/s. The reduction is progressively reduced at high operating feed flow rate of $2.43\text{E-}3$ m³/s as can be seen in Figure 6.73.

Despite at the fact that high operating pressures would help the water flux, the impact of running the process at low feed flow rate is that the concentration polarisation is increased, and this can be used as a control feature of the system. In other words, when the solute flux through the membrane is increased, the NDMA rejection is reduced. The main conclusion here is that using a higher feed flow would be preferable for improving the NDMA removal. This conclusion is illustrated in both Figures 6.72 and 6.73, whereby an increase of the feed flow rate can reinforce the mass transfer coefficient and periodically improve the NDMA rejection.

The effect of feed flow rate and concentration variations of $7.85\text{E-}4$ to $2.5\text{E-}3$ m³/s and $74.1\text{E-}6$ to $370\text{E-}6$ ppm, respectively, for three different cases of fixed operating pressure of 6.51, 10, and 18 atm, at constant temperature of 20 °C on NDMA rejection is highlighted in Figures 6.74, 6.75, and 6.76, respectively. Figure 6.77 shows

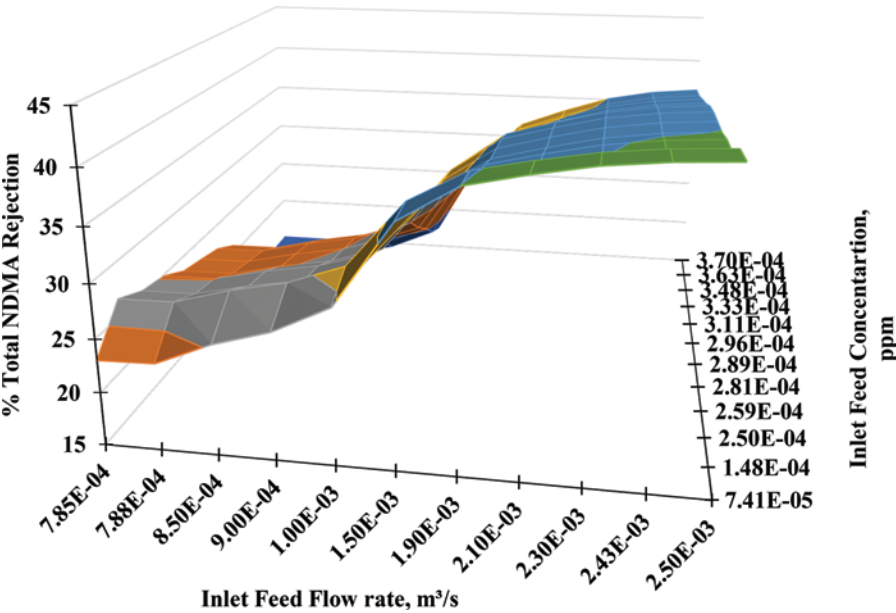


FIGURE 6.74 Impact of variation in feed concentration and flow rate on total NDMA rejection at fixed inlet feed pressure and temperature (6.51 atm and 20 °C).

(Adapted from Al-Obaidi et al., 2017e)

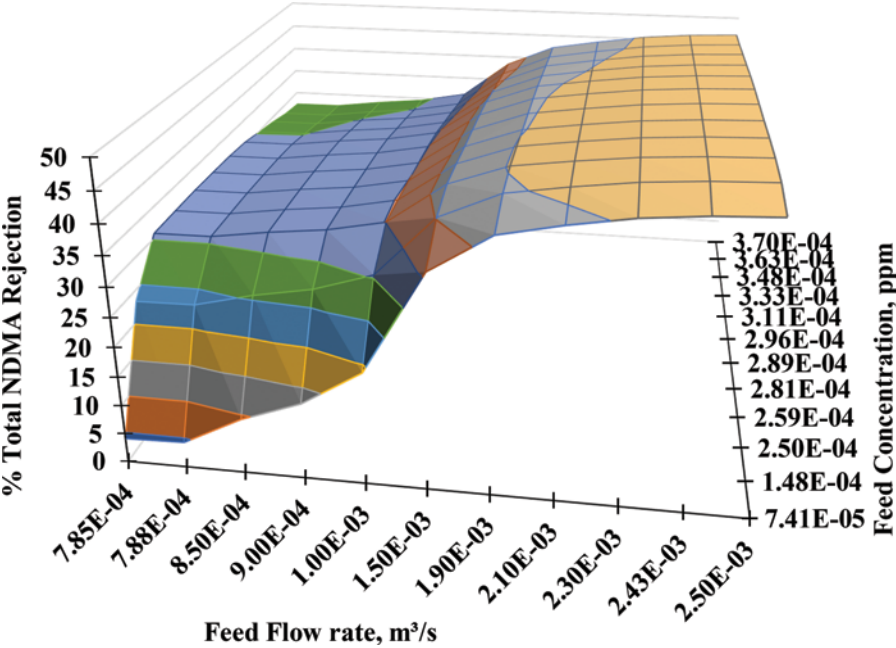


FIGURE 6.75 Impact of variation in feed concentration and flow rate on total NDMA rejection at fixed inlet feed pressure and temperature (10 atm and 20 °C).
(Adapted from Al-Obaidi et al., 2017e)

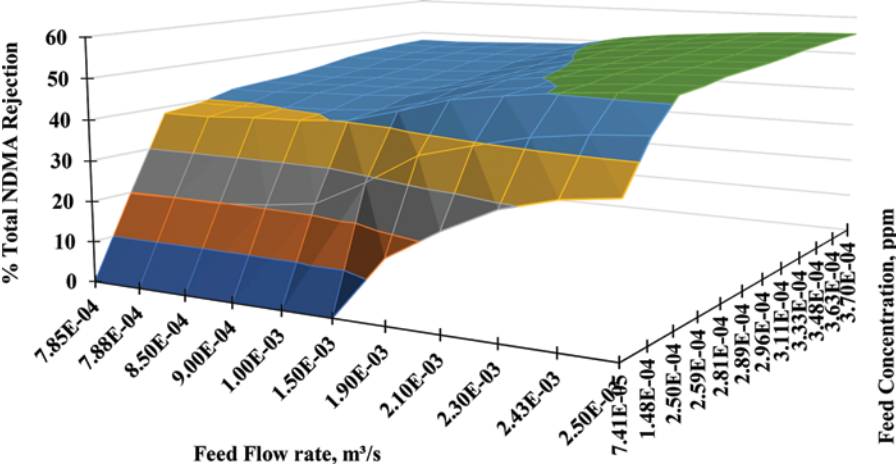


FIGURE 6.76 Impact of variation in feed concentration and flow rate on total NDMA rejection at fixed inlet feed pressure and temperature (18 atm and 20 °C).
(Adapted from Al-Obaidi et al., 2017e)

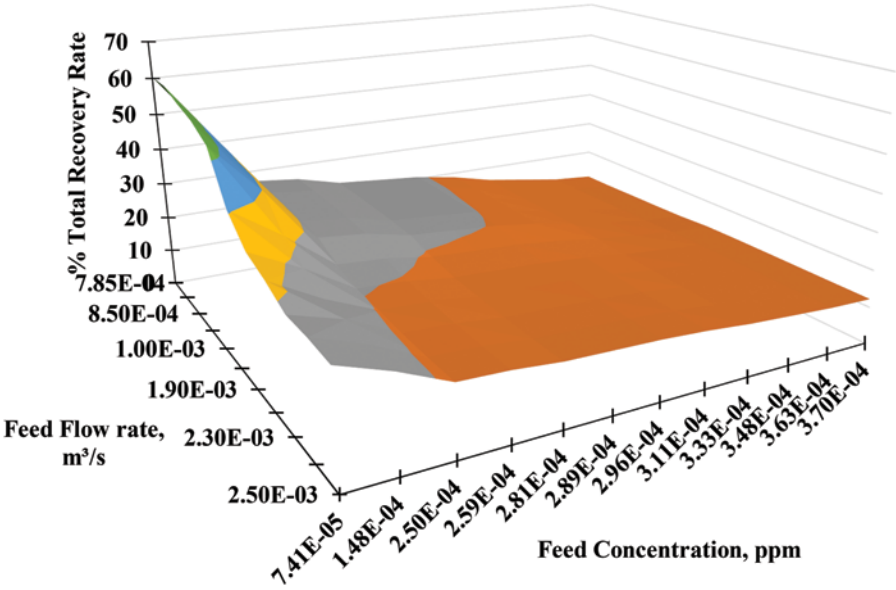


FIGURE 6.77 Impact of variation in feed concentration and flow rate on total recovery rate at fixed feed pressure and temperature (10 atm and 20 °C).

(Adapted from Al-Obaidi et al., 2017e)

the impact of the same variation of feed flow rate and concentration on the water recovery at the fixed pressure and temperature of 18 atm and 20 °C, respectively.

Figures 6.74 and 6.75 confirm the optimum NDMA rejection of 42.87% and 48.49%, respectively, for the range of operating pressures tested at 6.5 and 10 atm, respectively. These optimum values are attained at the operating conditions of a feed flow rate of 2.5E-3 m³/s and concentrations of 74.1E-6 ppm and 250E-6 ppm, corresponding to the operating pressure of 6.51 and 10 atm, respectively. In line with these findings, Figure 6.76 confirms a maximum NDMA rejection of 55.4% attained at 370E-6 ppm. This was at an operating pressure of 18 atm and a feed flow rate of 2.5E-3 m³/s, which confirms that the optimum NDMA rejection is always obtained at the highest feed flow rate regardless of the operating pressure.

Figure 6.74 shows the reduction of NDMA rejection at about 14.8%, from 42.87% to 36.5%, due to the increase of feed concentration from 74.1E-6 ppm to 250E-6 ppm. A noticeable increase in NDMA rejection of about 85.9%, from 23% to 42.87%, is observed due to the increase of the feed flow rate from 7.85E-4 m³/s to 2.5E-3 m³/s. Figure 6.74 indicates that the maximum NDMA rejection for the low operating pressure tested at 6.51 atm is attained at the lowest concentration used. This is due to absence of the concentration polarisation at the lower feed concentrations, and which in turn causes an increase in the water flux, as clearly indicated in Figure 6.77. This affirms that the highest water recovery is achieved at the lowest feed concentration for all the feed flow rates tested for the same aforementioned reason. Figure 6.77 indicates that the feed flow rate has a significant effect on water recovery at the

lowest range of feed concentrations. Figure 6.75 shows that the maximum NDMA rejection is attained at a feed concentration of $250\text{E-}6$ ppm and $2.5\text{E-}3$ m³/s, when the pressure applied is increased to 10 atm. This again confirms the feed flow rate and concentration can in fact be used to control the NDMA rejection at the middle range of operating pressures. The increase of feed flow rate, from $7.85\text{E-}4$ m³/s to $2.5\text{E-}3$ m³/s, causes an increase of the NDMA rejection by 57.7% from 30.74% to 48.49%, where $2.5\text{E-}3$ m³/s is essentially the optimum feed flow rate for a maximum rejection of 48.49% (Figure 6.75). The maximum NDMA rejection occurs at a specific optimum concentration for the case of 10 atm compared to that of the low pressure of 6.51 atm, as shown in Figures 6.74 and 6.75. Interestingly, the operating conditions associated with the maximum NDMA rejection represent the lowest water recovery that can possibly be achieved (Figure 6.77).

Figure 6.76 indicates that the increase of the feed concentration from $74.1\text{E-}6$ ppm to $370.25\text{E-}6$ ppm causes around 63% improvement on the NDMA rejection, with $370.25\text{E-}6$ ppm representing the optimum concentration with the highest rejection of 55.4%. There is a noticeable positive impact when increasing the feed flow rate from $7.85\text{E-}4$ m³/s to $2.5\text{E-}3$ m³/s, in that it causes a 16.6% increase on the NDMA rejection, with $2.5\text{E-}3$ m³/s being the optimum flow rate for maximum NDMA rejection. Additionally, an insignificant effect of the feed flow rate on the total water recovery is noticed when running the process at the operating conditions of 18 atm and $370.25\text{E-}6$ ppm and the variation of feed flow rate from $7.85\text{E-}4$ to $2.5\text{E-}3$ m³/s, where the recovery rate attained is approximately 24%.

Figures 6.75 and 6.76 clearly represent a significant drop in NDMA rejection when the process is running at the low feed flow rates of $7.85\text{E-}4$ to $1.5\text{E-}3$ m³/s and the low concentration despite the high operating pressures of 10 and 18 atm. This is attributed to the gradual solute accumulation on the membrane wall at the low feed flow rate conditions, which in turn rises the solute flux and reduces the water flux, thus lowering the NDMA concentration at the permeate channel. However, the NDMA rejection is significantly increased at a feed flow rate of $1.5\text{E-}3$ m³/s for all the operating concentrations tested.

Broadly speaking, increasing the operating concentration and flow rate decrease the water recovery, as particularly illustrated in Figure 6.77. In this respect, the increase of the concentration from $74.1\text{E-}6$ ppm to $370.25\text{E-}6$ ppm and the flow rate from $7.85\text{E-}4$ m³/s to $2.5\text{E-}3$ m³/s (the optimum operating conditions for maximum water recovery being $74.1\text{E-}6$ ppm and $7.85\text{E-}4$ m³/s) causes a noticeable decrease in water recovery to around 81% and 53%. This can be attributed to the increase of the osmotic pressure due to the increasing concentration and the reduced residence time of the bulk feed inside the modules.

Figure 6.78 shows the growth of the NDMA rejection through the seven RO elements of the full-scale plant given the operating conditions of a feed flow rate of $7.85\text{E-}4$ to $2.5\text{E-}3$ m³/s at constant feed concentration, pressure, and a temperature of $250\text{E-}6$ ppm, 10 atm, and 20 °C, respectively. It is fair to say that the NDMA rejection actually reduces along the series RO membranes for the set of operating feed flow rates. This is because of the changes occurring in the hydrodynamic states and solution properties in the subsequent feed and permeate channels. Indeed, Figure 6.78 affirms the importance of using high feed flow rate to boost the NDMA rejection as in the proposed configuration of Fujioka et al. (2014).

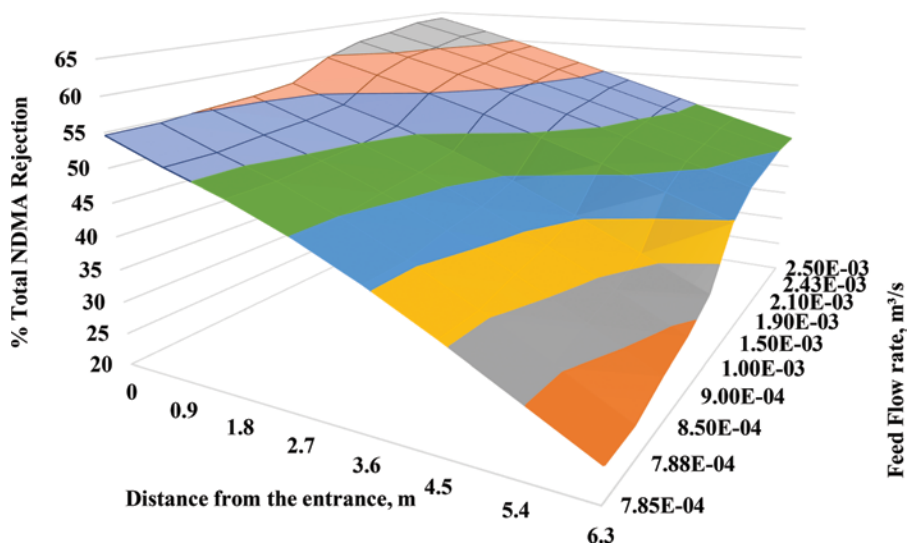


FIGURE 6.78 The progress of NDMA rejection along a series of seven RO elements (inlet feed conditions: 10 atm, 250E-6 ppm, and 20 °C).

(Adapted from Al-Obaidi et al., 2017e)

6.5 DYNAMIC SIMULATION: SENSITIVITY ANALYSIS OF THE OPERATING PARAMETERS

One characteristic of any industrial process is the possibility of a sudden or a sustained step change in the input parameters, which causes a corresponding change in the process performance. Moreover, the water flux loss in an RO membrane is a dynamic phenomenon. This therefore requires the use of an appropriate dynamic model for predicting the long-term water flux loss caused by membrane deterioration. This means that a fuller understanding of the process dynamics is essential as a pre-step for designing an effective controller system. These are required to reduce the fluctuation of the controlled parameters. The following sections present some of the successful examples of RO process used to explore the dynamic behaviour of the operating conditions for the removal of organic compounds from wastewater.

6.5.1 REMOVAL OF MULTIPLE SOLUTES FROM A PALM OIL MILL EFFLUENT USING RO PROCESS

Ahmad et al. (2007) developed a robust dynamic model (Model II, Chapter 5) based on the irreversible thermodynamic principles of an extended version of the Spiegler-Kedem model coupled with the concentration polarisation model with the inclusion of solute–solute interactions. This combined model was used to analyse the dynamic behaviour and transport phenomena of the RO process for removing complex organic matters of multiple solutes from a palm oil mill effluent. This particular effluent contained a ternary system of carbohydrate constituents, protein, and ammoniacal

nitrogen. Model predictions were compared to experimental data and confirmed its consistency. Figure 6.79 presents a schematic diagram of the RO process used. The variations of several operating conditions are analysed in the following sections.

The unsteady state simulation of the wall concentration of carbohydrate on the boundary layer against the operation time is depicted in Figure 6.80. This shows a sharp response at the initial filtration time which gradually attains its steady state. Also, Figure 6.80 illustrates the increase of the wall concentration of carbohydrate as a response to increasing the operating pressure. The rejection of carbohydrates increases with the operating time, which causes an increase in its wall concentration on the membrane surface and back-diffusion mass transfer rate into the boundary layer. These same behaviours occur for the other organic matters of protein and ammoniacal nitrogen. It is therefore fair to expect a reduction of water flux when increasing the build-up of carbohydrate concentration on the membrane surface as noted in Figure 6.81. This demonstrates the corroboration between experimental data and simulation results.

The unsteady state permeate concentrations of carbohydrate, protein, and ammoniacal nitrogen, at the operating pressures of 13.5 bar and 35 bar, are plotted against the operation time in Figures 6.82 and 6.83 respectively. These confirm a reduction of permeate concentration of each pollutant with the operating pressure, which increases the rejection due to higher water flux through the membrane. These figures also demonstrate a slight increase of permeate concentration at the initial operating time until the steady state value is reached.

Figure 6.84 shows the dynamic simulation of the intrinsic rejection of carbohydrate against the treatment time for a given set of operating pressures. The intrinsic rejection is increased due to the reduction of permeate concentration and an increase of the water flux and feed pressure.

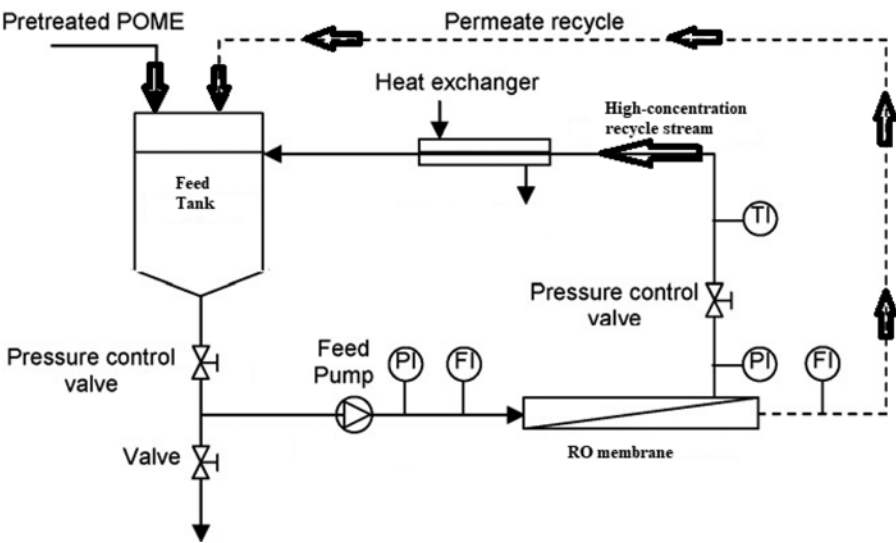


FIGURE 6.79 Schematic diagram of RO process.

(Adapted from Ahmad et al., 2007)

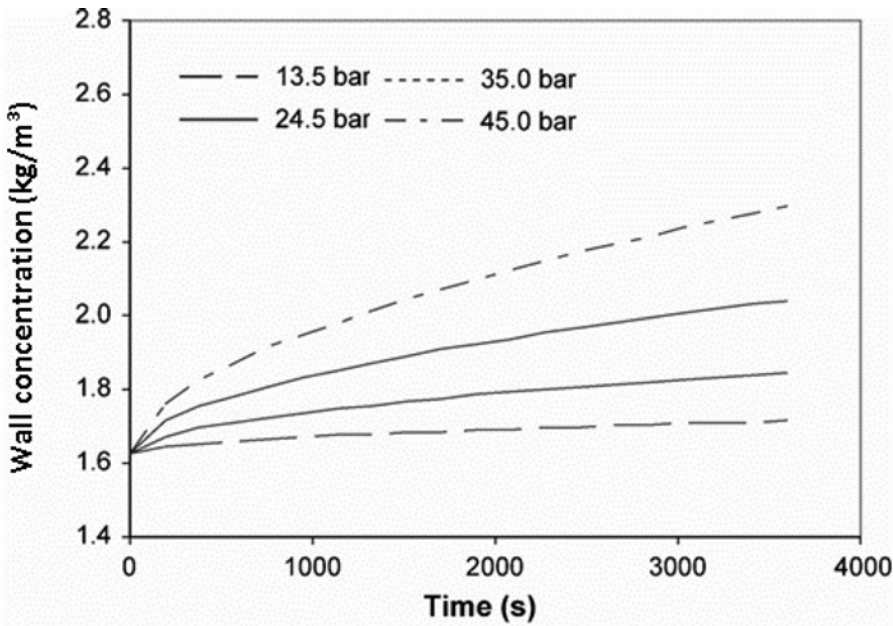


FIGURE 6.80 Unsteady state wall concentration of carbohydrate against treatment time at different operating pressures.

(Adapted from Ahmad et al., 2007)

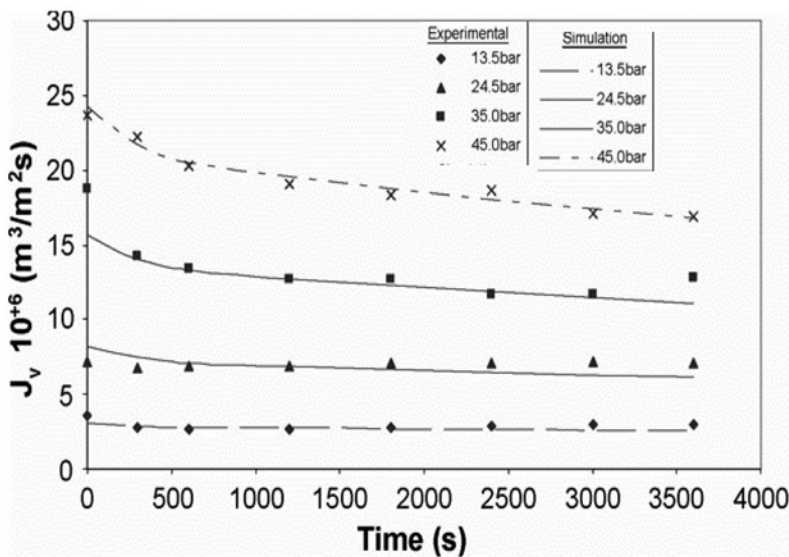


FIGURE 6.81 Experimental data and model predictions of water flux against treatment time at different operating pressures.

(Adapted from Ahmad et al., 2007)

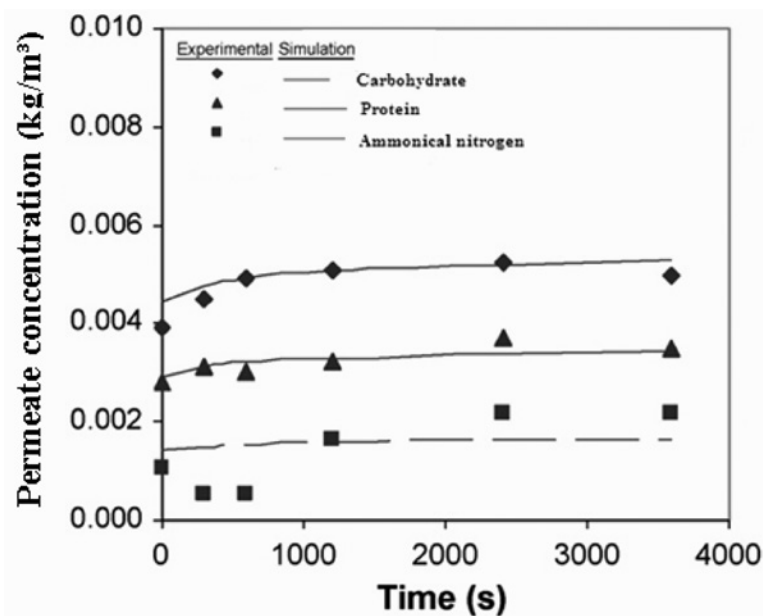


FIGURE 6.82 Experimental data and model predictions of permeate concentration of different solutes against treatment time at 35 bar.

(Adapted from Ahmad et al., 2007)

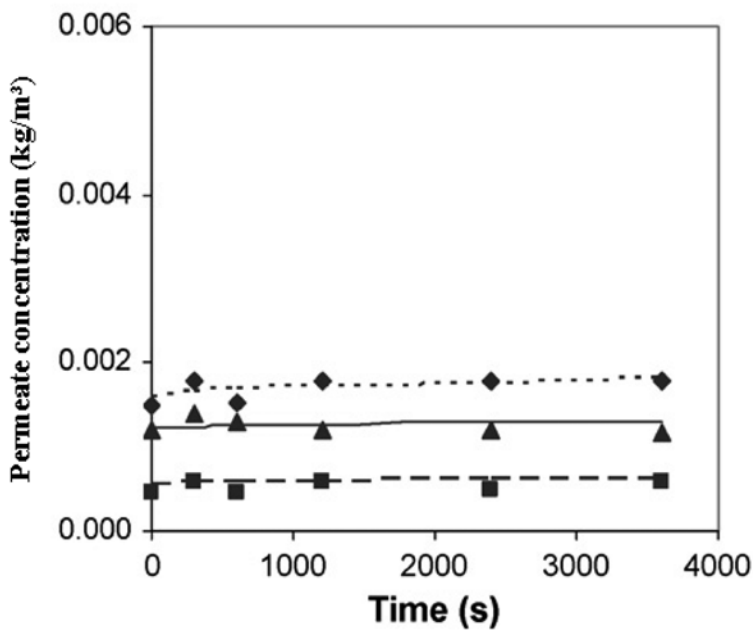


FIGURE 6.83 Experimental data and model predictions of permeate concentration of different solutes against treatment time at 13.5 bar.

(Adapted from Ahmad et al., 2007)

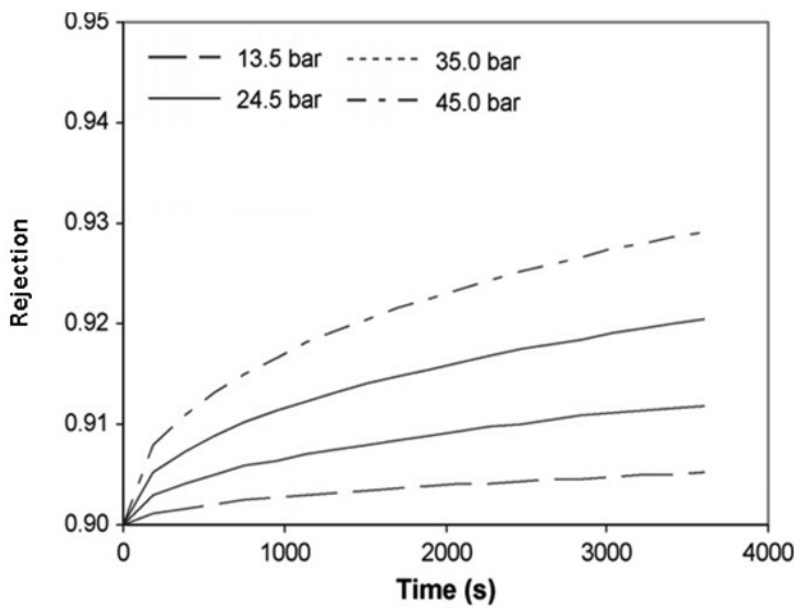


FIGURE 6.84 Model predictions of carbohydrate rejection against treatment time at different feed pressures.

(Adapted from Ahmad et al., 2007)

**6.5.2 THE REMOVAL OF CHLOROPHENOL FROM WASTEWATER
IN AN INDIVIDUAL SPIRAL WOUND RO PROCESS**

Al-Obaidi and Mujtaba (2016) analysed the dynamic behaviour of an individual spiral wound RO process via simulation using Model VII (Chapter 5). The dynamic version of their model is used to analyse the process performance under a considerable variation of operating parameters.

6.5.2.1 Effect of Inlet Feed Pressure

The dynamic behaviour of the chlorophenol removal from wastewater by a spiral wound RO process is depicted in Figures 6.85 and 6.86. These figures show a step change in the operating pressure and the responses of the average permeate concentration and solute rejection for two different feed flow rates at fixed feed concentration and temperature. Specifically, the operating pressure was 5.83 atm up to $t = 1800$ s, while the pressure increased to 13.58 atm at $t = 1800$ s. This causes a reduction of the average chlorophenol permeate concentration when the water flux is increased (Figure 6.85). This can improve the permeate concentration as well as increase the retentate concentration. Additionally, increasing the feed flow rate reduces the average permeate concentration due to the reduction of concentration polarisation.

The system needs about 300 to 400 s to reach its steady state conditions for the two feed flow rates as a response to the change of the operating pressure (Figures 6.85

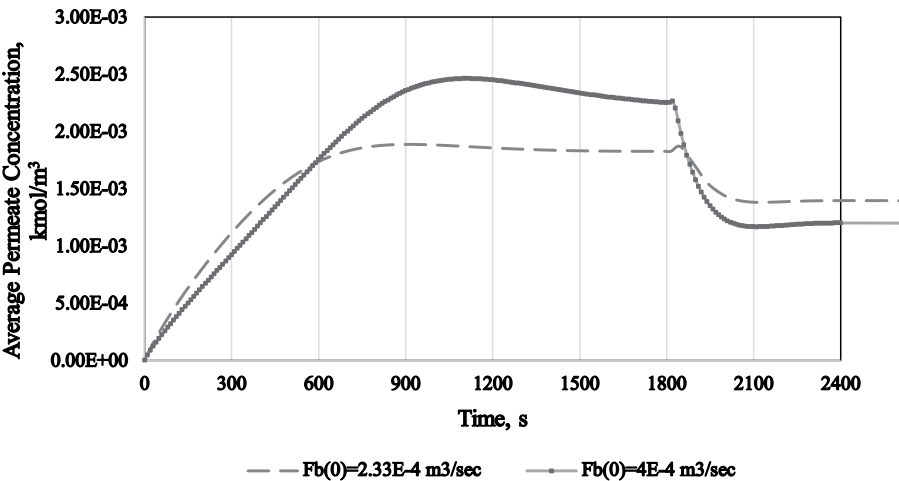


FIGURE 6.85 Impact of step changes in inlet feed pressure on average permeate concentration of different inlet feed flow rates (inlet feed conditions, $6.226E-3$ kmol/m³, and 31°C). (Adapted from Al-Obaidi and Mujtaba, 2016)

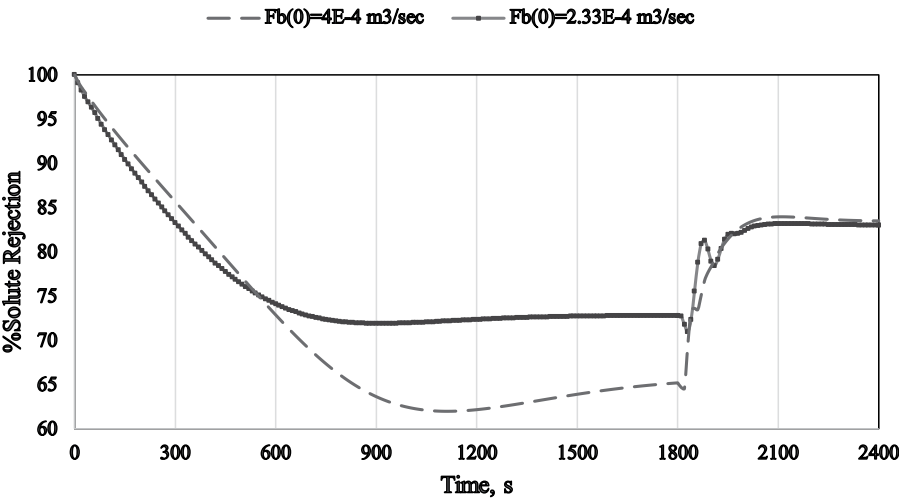


FIGURE 6.86 Impact of step changes in inlet feed pressure on %solute rejection of different inlet feed flow rates (inlet feed conditions, $6.226E-3$ kmol/m³, and 31°C). (Adapted from Al-Obaidi and Mujtaba, 2016)

and 6.86). However, the settling time for the high feed flow rate is a bit longer than the low feed flow rate (before and after the step change in pressure). This is because the higher feed flow rate tends to lower the residence time (for a given volume). The reduction of chlorophenol rejection at high inlet feed flow rate is more noticeable when compared to a low feed flow rate (Figure 6.86) at a low operating pressure

of 5.83 atm. The reduction of the water flux due to the increasing feed flow rate can possibly explain this phenomenon. However, the same increasing trend of chlorophenol rejection is noticed for both feed flow rates at the high operating pressure of 13.58 atm. The high feed flow rate corresponds to a slightly higher chlorophenol rejection and a bigger overshoot compared to that at the lower feed flow rate.

Figure 6.86 confirms that the step change in pressure results in an insignificant transient response in chlorophenol rejection at high feed flow rate compared to low feed flow rate. The high pressure and high flow rate conditions cut down the disturbance time and the required time to settle the retentate concentration. These conditions essentially help reduce the time for the retentate concentration to reach its steady state (Figure 6.87).

The bulk concentration has a major impact on the chlorophenol rejection response. In this respect, Figure 6.86 shows relatively little overshoot and undershoot in the response of chlorophenol rejection after increasing the operating pressure at a low feed flow rate before reaching a new steady state value. The dynamic equations of the feed and permeate solute concentrations of the model by Al-Obaidi and Mujtaba (2016) can be used to understand this phenomenon. Clearly, the feed concentration equation has a disturbance variable (feed flow rate) compared to the output variable (permeated flow rate) in the average permeate concentration equation. It is therefore fair to say that any disturbance of the operating pressure, temperature, and feed flow rate at steady state will directly impact the bulk and retentate concentrations. It is therefore fair to expect the retentate concentration to this disturbance would take some time until it reaches a new steady state value (Figure 6.87). However, Figure 6.85 shows that the response of an average permeate concentration is not directly affected by this step change of operating pressure for both the feed flow rates tested. More importantly, the response of the chlorophenol rejection at the transient

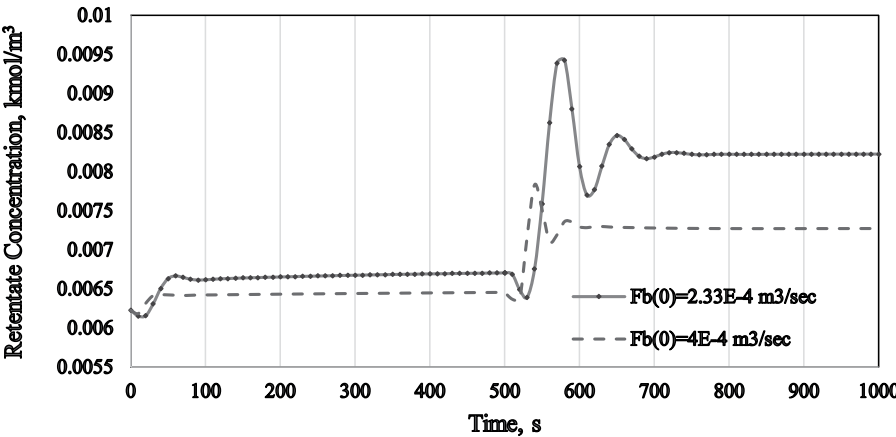


FIGURE 6.87 Impact of step changes in inlet feed pressure on outlet brine concentration of different inlet feed flow rates (inlet feed conditions, 6.226E-3 kmol/m³, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

time will be somewhat similar to retentate concentration trajectory due to having both the retentate and permeate concentrations in the rejection equation.

6.5.2.2 Effect of Inlet Feed Flow Rate

The dynamic responses of two step changes in the inlet feed flow on the average permeate concentration and solute rejection are depicted in Figures 6.88 and 6.89, respectively, for two different initial feed pressures at fixed feed concentration and temperature. The inlet feed flow rate was $2.33\text{E-}4\text{ m}^3/\text{s}$ up to $t = 1000\text{ s}$, and was then increased to $2.583\text{E-}4\text{ m}^3/\text{s}$ at $t = 1000\text{ s}$ for the first step change. However, for the second step change, the inlet feed flow rate was $2.583\text{E-}4\text{ m}^3/\text{s}$ up to $t = 1500\text{ s}$, and was then increased to $4.0\text{E-}4\text{ m}^3/\text{s}$ at $t = 1500\text{ s}$.

The system clearly needed between 250 and 350 s to reach its steady state during the inlet feed flow rate step changes.

Figure 6.88 shows that the reduction of permeate chlorophenol concentration is inversely comparable to the low and high inlet feed pressures of 7.77 and 13.58 atm. The low operating pressure and the highest feed flow rate actually increase the permeate concentration of chlorophenol (Figure 6.88), and the reason for this is the reduction of residence time and the use of the lowest pressure. Also, it is fair to say that increasing the inlet feed flow rate increases the frictional pressure drop that retards the water flux and finally increases the average permeate concentration. This then decreases the chlorophenol rejection at these operating conditions (Figure 6.89). Another interesting phenomenon can be seen in Figure 6.88. The use of the high operating pressure and feed flow rate conditions in the second step change causes a reduction of the average permeate chlorophenol concentration. This time, the system

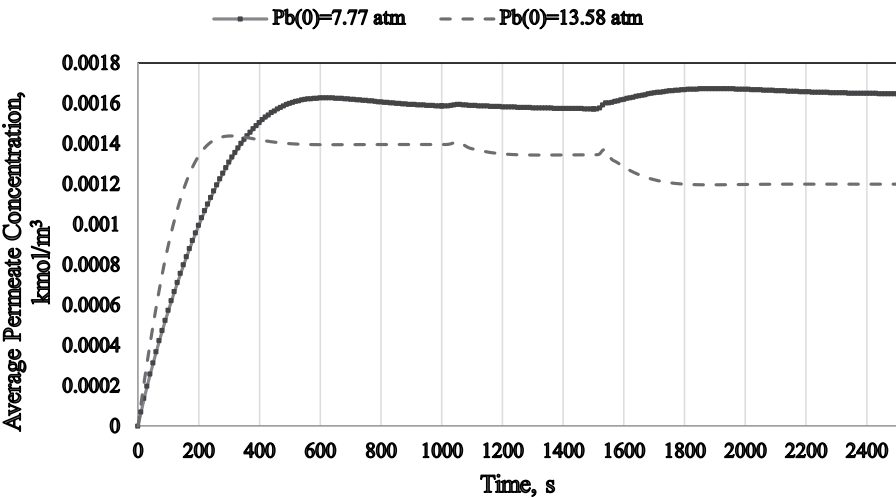


FIGURE 6.88 Impact of step changes in inlet feed flow rate on average permeate concentration of different inlet feed pressures (inlet feed conditions, $6.226\text{E-}3\text{ kmol/m}^3$, and $31\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi and Mujtaba, 2016)

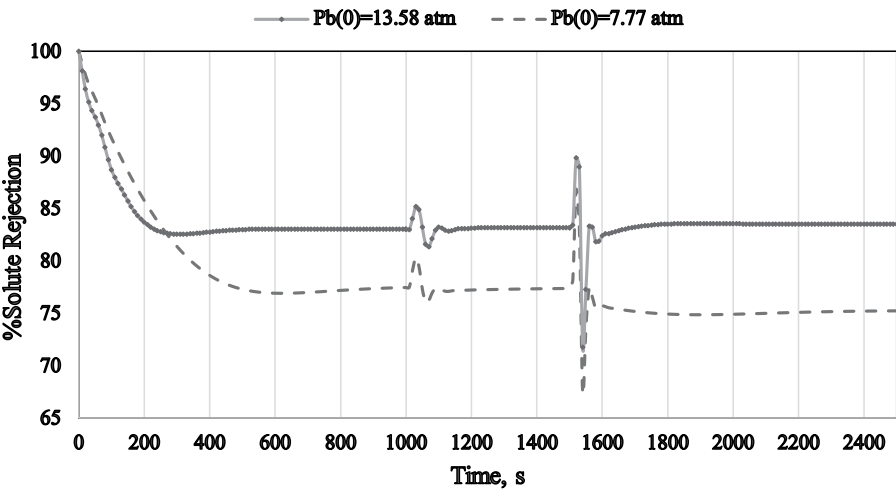


FIGURE 6.89 Impact of step changes in inlet feed flow rate on %solute rejection of different inlet feed pressures (inlet feed conditions, $6.226\text{E-}3\text{ kmol/m}^3$, and $31\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi and Mujtaba, 2016)

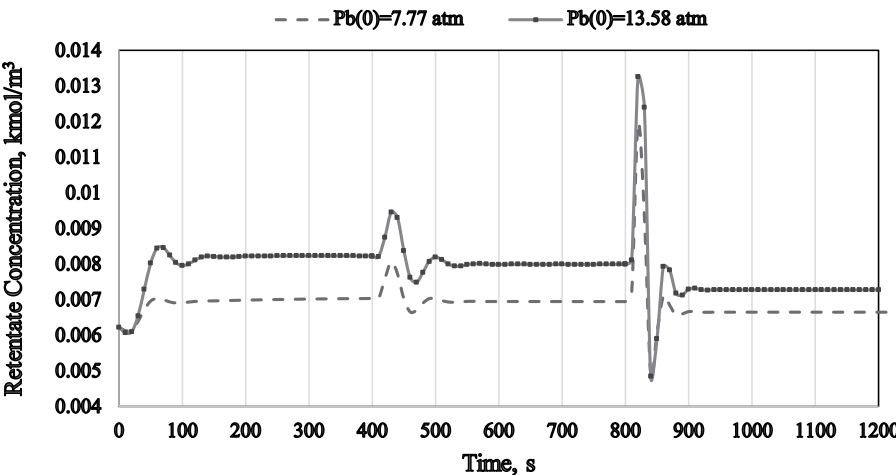


FIGURE 6.90 Impact of step changes in inlet feed flow rate on outlet brine concentration of different inlet feed pressures (inlet feed conditions, $6.226\text{E-}3\text{ kmol/m}^3$, and $31\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi and Mujtaba, 2016)

requires a longer time to settle when using a high inlet feed flow rate in the second step change compared to the first one. This can be explained by the increase of the rate of instability throughout the second step change.

Figure 6.90 shows that increasing the operating feed flow rate has a positive impact on decreasing the retentate chlorophenol concentration for the two step

changes considered. This can be attributed to the reduction of concentration polarisation and the associated increase in the mass transfer coefficient due to lifting the feed flow rate. Figure 6.90 shows another interesting aspect in that the retentate concentration increases rapidly, then reduces sharply immediately after the step change is applied in the feed flow rate, and finally reaches a new steady state after about 150 s. However, the response is sharper and more rapid (noticeable) for the second step change. It can therefore be said that the response of the retentate chlorophenol concentration is much faster than that of the average permeate chlorophenol concentration transient.

6.5.2.3 Effect of Inlet Feed Concentration

The dynamic simulation of two step changes in the inlet feed chlorophenol concentration on the average permeate concentration and solute rejection are depicted in Figures 6.91 and 6.92, respectively, for two different initial feed pressures at fixed feed concentration and temperature.

Specifically, the inlet feed chlorophenol concentration was $0.778\text{E-}3\text{ kmol/m}^3$ up to $t = 1000\text{ s}$, and it then increased to $2.335\text{E-}3\text{ kmol/m}^3$ at $t = 1000\text{ s}$ for the first step change. However, for the second step change, the feed concentration was $2.335\text{E-}3\text{ kmol/m}^3$ up to $t = 2000\text{ s}$, and it then increased to $6.226\text{E-}3\text{ kmol/m}^3$ at $t = 2000\text{ s}$.

It is fair to expect that when the operating concentration is increased, it would trigger an increase of the osmotic pressure, solute flux, and associated chlorophenol concentration at the permeate channel, as more particularly illustrated in Figure 6.91. This shows that the system requires less time to settle when using a high operating pressure compared to when using a low operating pressure. The system needs between 500 and 600 s to reach a new steady state in both the two

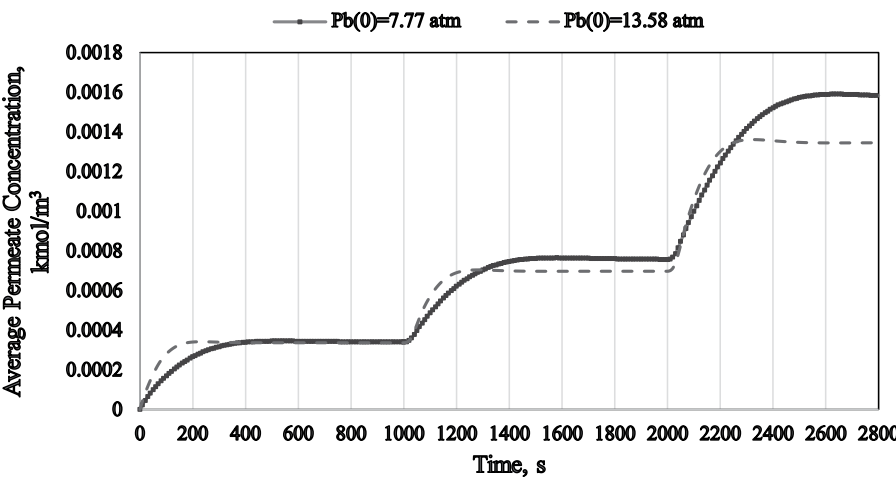


FIGURE 6.91 Impact of step changes in inlet feed concentration on average permeate concentration of different inlet feed pressures (inlet feed conditions, $2.583\text{E-}4\text{ m}^3/\text{s}$, and $31\text{ }^{\circ}\text{C}$).

(Adapted from Al-Obaidi and Mujtaba, 2016)

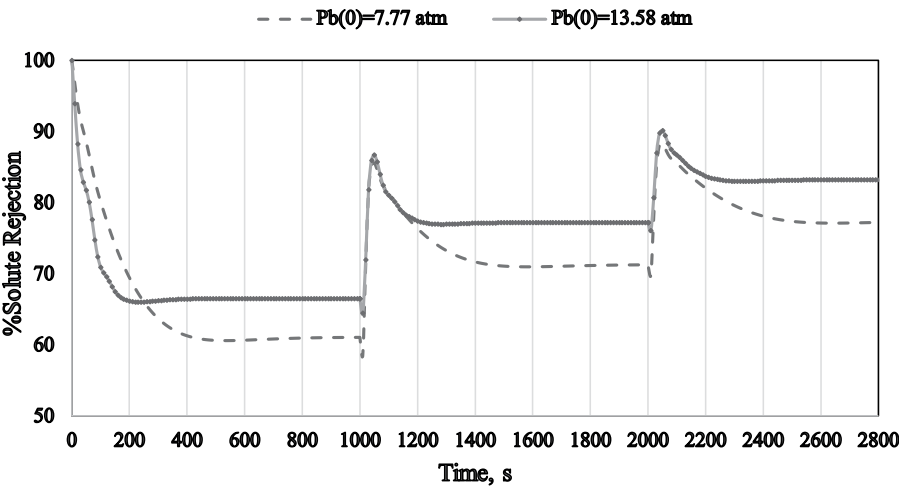


FIGURE 6.92 Impact of step changes in inlet feed concentration on %solute rejection of different inlet feed pressures (inlet feed conditions, 2.583E-4 m³/s, and 31 °C).

(Adapted from Al-Obaidi and Mujtaba, 2016)

step changes when the low operating pressure is applied (Figures 6.91 and 6.92). In the case of high operating pressure, the system requires a shorter time, typically between 300 and 400 s, to settle. The use of a high operating pressure increases the level of water permeation through the membrane, thus resulting in a faster fixed average permeate chlorophenol concentration than that observed for a low operating pressure.

Figure 6.92 shows that the chlorophenol rejection is increased when the concentration is increased. The same behaviour was also observed by Tabassi et al. (2014) for the removal of phenol from wastewater. Figure 6.92 shows a small undershoot and then a larger overshoot of the chlorophenol rejection for the step changes in the feed concentration. The first response resulted in the longest shoot compared to the second response and that the first step change is bigger than the second one. These behaviours are linked to the retentate concentration response as more particularly illustrated in Figure 6.90. The chlorophenol rejection response at the high operating pressure resulted in a slight undershoot compared to the one made at the low operating pressure. The difference of water flux in these two cases can explain the reason why the increase of the operating pressure is sufficient to increase the chlorophenol rejection.

6.5.3 REMOVAL OF DIMETHYLPHENOL FROM WASTEWATER IN AN INDIVIDUAL SPIRAL WOUND RO PROCESS

Al-Obaidi et al. (2018b) explored the unsteady hydrodynamics and the sensitivity of an individual spiral wound RO process for the removal of dimethylphenol from wastewater using the dynamic version of Model VIII. This provided a clear

explanation of the dynamic response of most process performance indicators against the variation of the operating conditions.

6.5.3.1 Inlet Feed Pressure

The dynamic impacts of a step change in the inlet feed pressure on the average retentate concentration, average permeate concentration, solute rejection, water recovery, and average retentate flow rate for a set of inlet feed concentrations at fixed feed flow rate and temperature are depicted in Figures 6.93 to 6.97. The inlet feed pressure was 9.71 atm $t = 600$ s, and it then increased by 40% to 13.58 atm at $t = 600$ s.

Figures 6.93 and 6.94 clearly show that increasing the operating pressure causes an increase in the average retentate concentration. This corresponds to a reduction in the average permeate concentration and causes an increase in the dimethylphenol rejection and water recovery, and a decrease in the retentate flow rate, for all the feed concentrations implemented, as more particularly shown in Figures 6.95, 6.96, and 6.97. Unquestionably, increasing the operating pressure increases the quantity of water penetrated through the membrane. An increase in the water flux is followed by a decrease of the retentate flow rate, an increase of the retentate concentration, and finally a decrease of the permeate concentration at the permeate channel due to a high level of dilution. The dimethylphenol rejection is therefore enhanced because of the improvement of the water flux.

The application of a step change in the operating pressure, as shown in Figures 6.94 and 6.95, results in a more visible response for the higher concentration solution than the lower one. At the higher one, the impact of concentration polarisation is larger than the lower concentrations. Therefore, any increase in the operating pressure results in a significant effect on the concentration polarisation

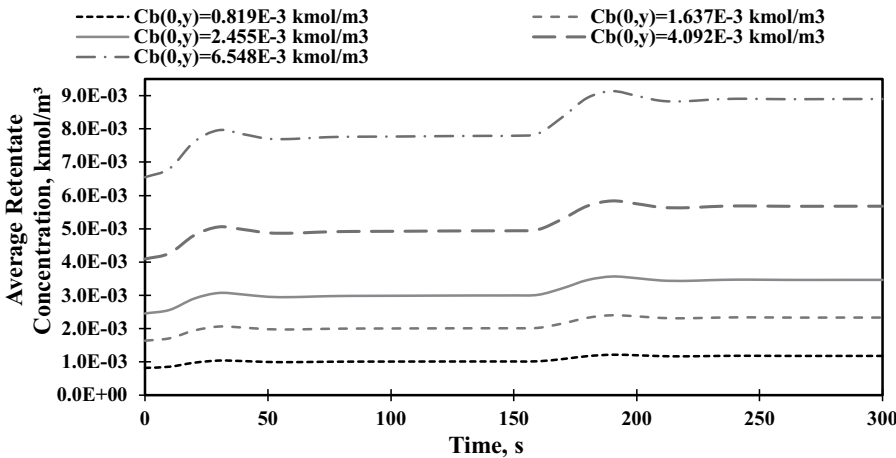


FIGURE 6.93 The result of the step change of operating pressure on retentate concentration for several operating concentrations at operating conditions of 2.583×10^{-4} m³/s, 9.71 atm, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

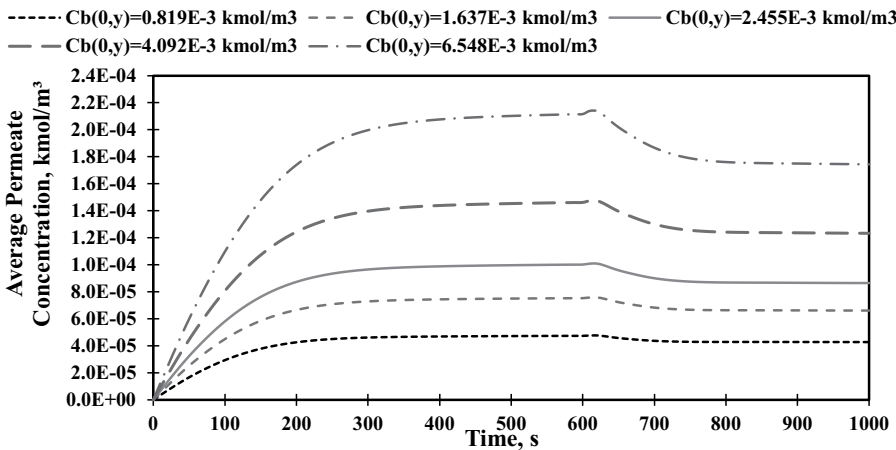


FIGURE 6.94 The result of the step change of operating pressure on mean permeate concentration for several operating concentrations at operating conditions of 2.583×10^{-4} m³/s, 9.71 atm, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

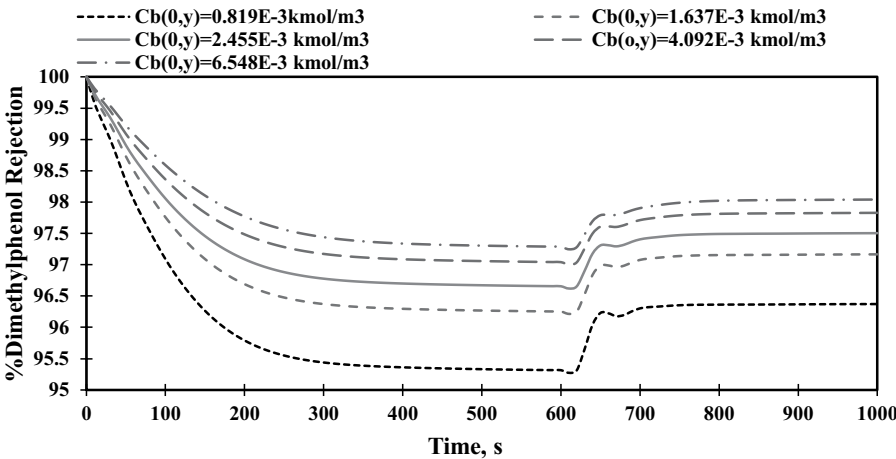


FIGURE 6.95 The result of the step change of operating pressure on solute rejection for several operating concentrations at operating conditions of 2.583×10^{-4} m³/s, 9.71 atm, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

and dimethylphenol concentration in both the feed and permeate channels, compared to other solutions of lower feed concentration. When applying an increase in the operating pressure, the system responds with a higher overshoot in the retentate concentration and a lower overshoot in the mean permeate concentration, as shown in Figures 6.95 and 6.94, respectively. Indeed, a unique underdamped response is

noted on the average permeate concentration (Figure 6.94), where it shows no overshoots before getting to the steady state condition. This is quite interesting when compared to other operating parameters tested where it shows slight but sharp overshoots. This explains the direct relationship that exists between the operating pressure step change and the feed channel. The feed flow rate and retentate concentrations are quickly affected compared to the permeate concentration at the permeate channel. This is why no sharp response with any overshoot can be seen at the permeate concentration.

The dimethylphenol rejection increases due to an increase in the inlet feed concentration (Figure 6.95), which can be attributed to two reasons. Despite increasing the inlet feed concentration causing an increase in the osmotic pressure and the permeate concentration, the increase of permeate concentration is insignificant with the increase of bulk concentration in the feed channel. Additionally, a rise of the membrane solute rejection intensity can be seen when the operating concentration increases. The research of Gómez et al. (2009) concluded the same findings for all the three types of membranes tested. The dimethylphenol rejection results in an overshoot due to its direct relation to both the retentate and permeate concentrations (Figure 6.94).

Figure 6.96 shows a reduction of water recovery when increasing the operating dimethylphenol concentration. This is caused by the declining level of water flux when the osmotic pressure is increased and which progresses with the feed concentration. Consequently, the retentate flow rate increases when the dimethylphenol operating concentration increases (Figure 6.97).

The implementation of a higher inlet feed concentration results in a longer settling time for an average permeate concentration (Figure 6.94) compared to that of a lower feed concentration. This is mostly because a higher solute concentration medium

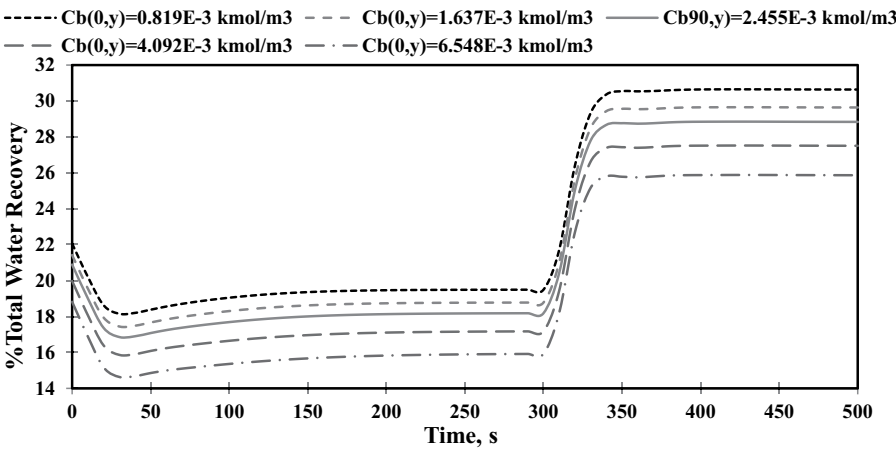


FIGURE 6.96 The result of the step change of operating pressure on total water recovery for several operating concentrations at operating conditions of 2.583×10^{-4} m³/s, 9.71 atm, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

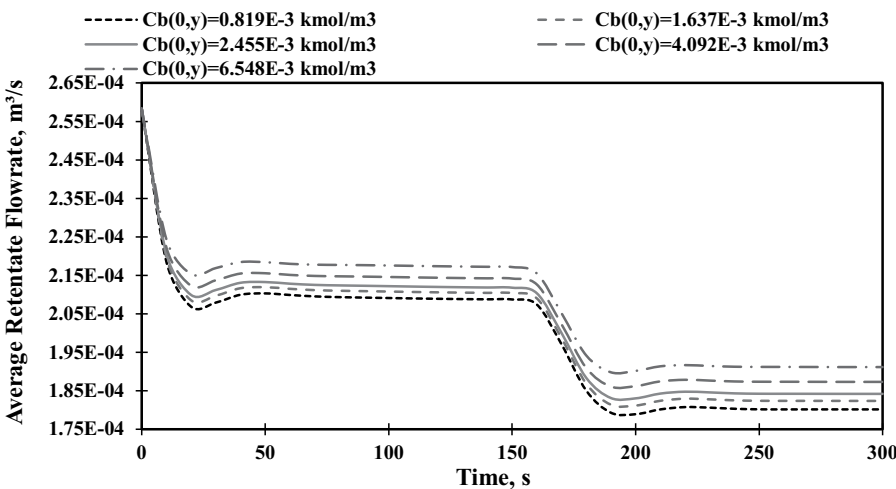


FIGURE 6.97 The result of the step change of operating pressure on retentate flow rate for several operating concentrations at operating conditions of 2.583×10^{-4} m³/s, 9.71 atm, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

requires more time to settle than the lower ones (for a given volume) and vice versa. Several observations can be noted in Figure 6.95 as follows.

- Between 200 s and 250 s are required to the reach the steady state dimethylphenol rejection for the set of feed concentrations, albeit with a little bit of a difference.
- The dimethylphenol rejection transient response of the lower feed concentration to the feed pressure step change is irrelevant compared with the one at a higher feed concentration. This is due to a higher water flux at a lower feed concentration medium compared to a higher feed concentration medium with a relative impact of concentration polarisation.

Al-Obaidi et al. (2018b) used the possibility of a ramped change of operating conditions, which is essentially carried out in a gradual upward or downward change for a period of time with a constant slope. In this respect, the response of dimethylphenol rejection towards a ramped change in the operating pressure is shown in Figure 6.98 at a fixed operating concentration, flow rate, and temperature. Up to $t = 600$ s, the inlet feed pressure is 10 atm and is then increased to 12, 14, and 16 atm, at 600, 900, and 1200 s, respectively.

It is clear that any increase of operating pressure increases the dimethylphenol rejection. However, Figure 6.98 shows that the ramped change of a 2 atm increase in the pressure has a relatively different settling time, where the process can be rapidly settled at higher operating pressures. This is owing to the increasing water flux with the increasing pressure, which ultimately decreases the settling time of permeate concentration at the permeate channel (Figure 6.99).

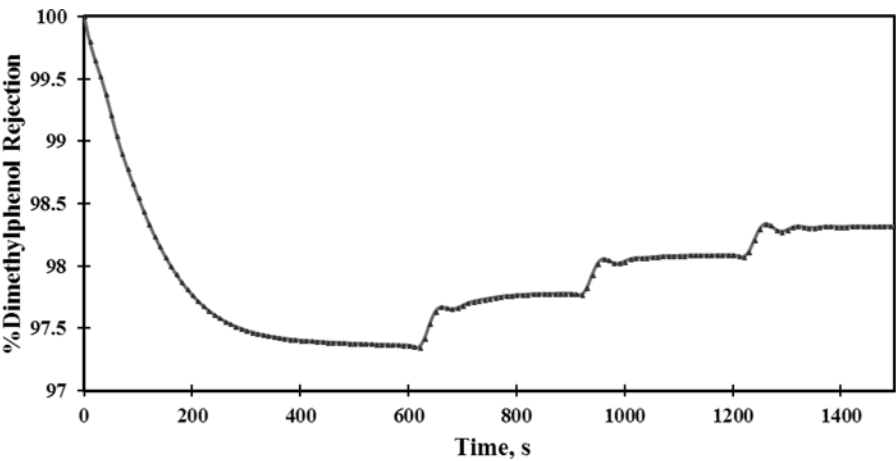


FIGURE 6.98 The result of the ramp change of operating pressure on solute rejection for operating conditions of 6.548×10^{-3} kmol/m³, 2.166×10^{-4} m³/s, 10 atm, and 31.5 °C. (Adapted from Al-Obaidi et al., 2018b)

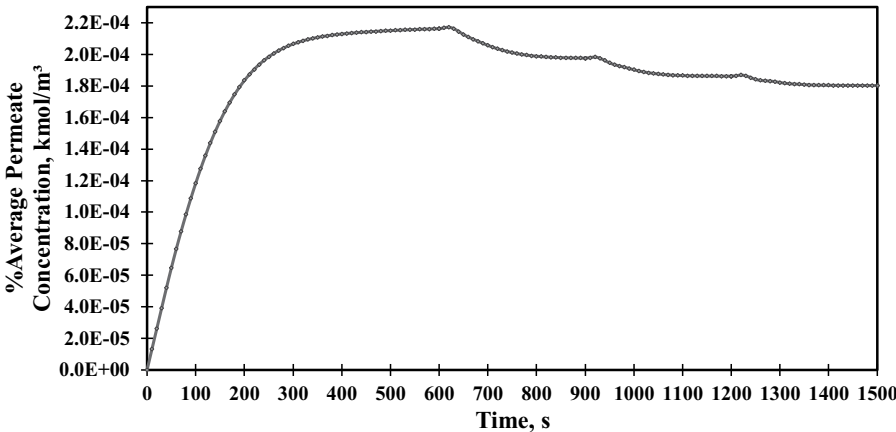


FIGURE 6.99 The result of the ramp change of operating pressure on average permeate concentration for operating conditions of 6.548×10^{-3} kmol/m³, 2.166×10^{-4} m³/s, 10 atm, and 31.5 °C. (Adapted from Al-Obaidi et al., 2018b)

6.5.3.2 Inlet Feed Flow Rate

The dynamic impacts of a step change in the inlet feed flow rate on the average retentate concentration, average permeate concentration, and solute rejection for a set of inlet feed pressure at fixed feed concentration and temperature are given in Figures 6.100 to 6.102, respectively. These figures are intentionally drawn with

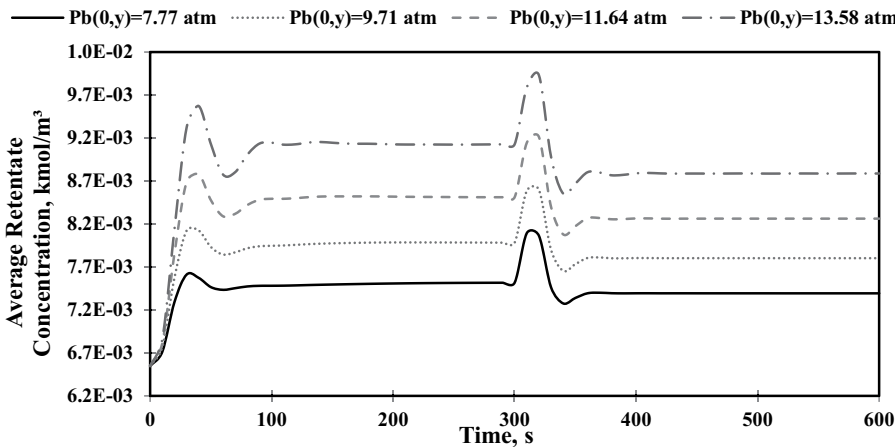


FIGURE 6.100 The influence of the step change of operating feed flow rate on retentate concentration for several operating pressures at operating conditions of $6.548 \times 10^{-3}\text{ kmol/m}^3$, $2.33 \times 10^{-4}\text{ m}^3/\text{s}$, and $31.5\text{ }^\circ\text{C}$.

(Adapted from Al-Obaidi et al., 2018b)

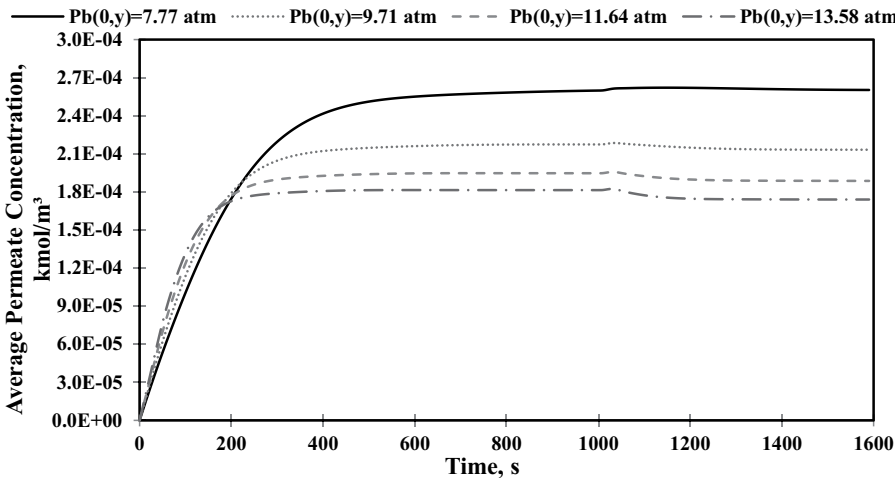


FIGURE 6.101 The influence of the step change of operating feed flow rate on average permeate concentration for several operating pressures at operating conditions of $6.548 \times 10^{-3}\text{ kmol/m}^3$, $2.33 \times 10^{-4}\text{ m}^3/\text{s}$, and $31.5\text{ }^\circ\text{C}$.

(Adapted from Al-Obaidi et al., 2018b)

different time axes to show the impact of the step change in a clearer way on the specific parameters.

Specifically, the inlet feed flow rate used was $2.33\text{E-}4\text{ m}^3/\text{s}$ up to $t = 1000\text{ s}$ and was then increased to $2.583\text{E-}4\text{ m}^3/\text{s}$ at $t = 1000\text{ s}$.

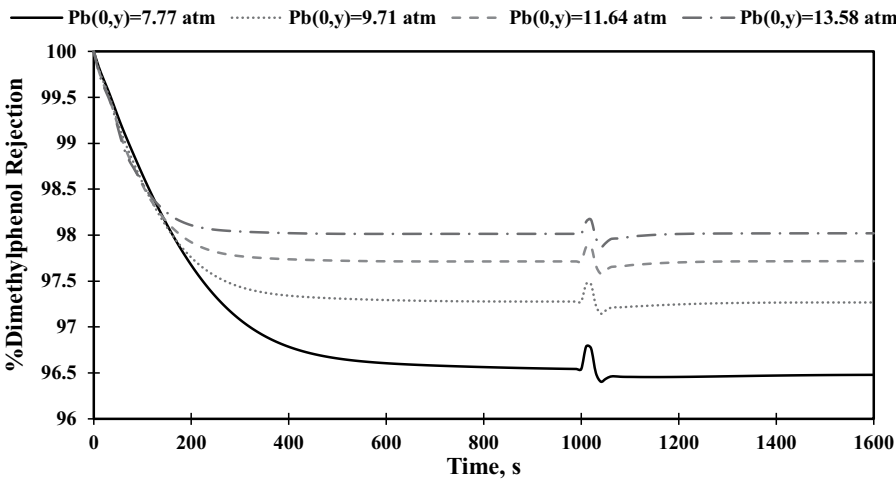


FIGURE 6.102 The influence of the step change of operating feed flow rate on rejection parameter for several operating pressures at operating conditions of $6.548 \times 10^{-3} \text{ kmol/m}^3$, $2.33 \times 10^{-4} \text{ m}^3/\text{s}$, and $31.5 \text{ }^\circ\text{C}$.
(Adapted from Al-Obaidi et al., 2018b)

One of the most important observations of this case is that the system has attained its steady state within 200 to 250 s after imposing the step change of the feed flow rate, which seems similar to the previous case of a step change of inlet pressure. The system response for the step change of operating flow rate results in a reduction of dimethylphenol concentration at both the feed and permeate channels. This is because any increase of the feed flow rate reduces the impact of concentration polarisation, which results in increasing the mass transfer coefficient.

It is obvious that the response in the retentate concentration as a result of a step change in the inlet feed flow rate results in a quick increase tracked by an instant high-pitched reduction before getting to a new steady state after about 150 s (Figure 6.100). However, a clear reduction in the retentate concentration occurs at a higher operating pressure. In this respect, the transient response of the average permeate concentration (Figure 6.101) is much slower than the corresponding response of the retentate concentration (Figure 6.100) for the same step change in the operating feed flow rate. Also, Figure 6.100 shows that implementing higher pressure conditions results in a higher degree of oscillation and overshoot (inverse response) in the response of the retentate concentration for a step change in the feed flow rate compared to a lower operating pressure that results in a slower response. The use of the higher inlet feed flow rate and operating pressure conditions can successfully reduce the dimethylphenol concentration along the feed channel compared to the use of lower pressure and higher feed flow rate conditions. It can therefore be said that a faster response, but without an overshoot, an average retentate concentration can be observed at very low operating pressures (Figure 6.100). Basically, the response of

the retentate concentration shown in Figure 6.100 is characterised by an increase followed by a significant decrease. The inverse response can be explained by increasing the feed velocity, which causes a reduction of residence time of the solution inside the medium, which increases the average retentate concentration due to its high disturbance. However, increasing the feed velocity causes a reduction of concentration polarisation with the operation time, which increases the mass transfer coefficient that finally retards the retentate concentration.

Figure 6.101 shows the response of the average permeate concentration where the use of high operating pressures causes a noticeable reduction in the average permeate concentration than that of low operating pressures. Increasing the water flux after increasing the pressure explains this phenomenon. Interestingly, Figure 6.101 shows an inverse but a slight increase of the average permeate concentration at low feed pressures compared to other feed pressures. This critical phenomenon can be attributed to the use of a low operating pressure (lower water flux) as well as an increase in the frictional pressure drop due to the increasing feed flow rate. This in turn reduces the advantage of osmotic pressure drop, which finally decreases the extent of water flux and lifts up the dimethylphenol concentration at the permeate channel. Based on the previous statement, the dimethylphenol rejection reduces as shown in Figure 6.102. The use of a high inlet feed flow rate and high operating pressure, however, helps reduce the average permeate concentration (Figure 6.101) and promotes the dimethylphenol rejection (Figure 6.102).

Al-Obaidi et al. (2018b) investigated the response of the treatment process for a ramped change of upward increase in the operating flow rate at constant other parameters, which is carried out for a period of time with different slopes as shown in Figures 6.103 to 6.105. In this respect, the inlet feed flow rate was $2.166\text{E-}4 \text{ m}^3/\text{s}$ up to $t = 500 \text{ s}$. However, the feed flow rate is increased to $4\text{E-}4 \text{ m}^3/\text{s}$ and $7\text{E-}4 \text{ m}^3/\text{s}$ at 500 and 1000 s, respectively. Figure 6.105 is intentionally drawn with different time axes than in Figures 6.104 and 6.105 to show the impact of the step change in a clearer way on the specific parameters.

Figure 6.103 shows that increasing feed flow rate by about 84% from $2.166\text{E-}4 \text{ m}^3/\text{s}$ to $4\text{E-}4 \text{ m}^3/\text{s}$ leads to substantial overshoot followed by an inverse response. However, the second ramped change is characterised by a low level of response after increasing the feed flow rate by 75% from $4\text{E-}4 \text{ m}^3/\text{s}$ to $7\text{E-}4 \text{ m}^3/\text{s}$. Increasing the feed flow rate for the first step change causes an instantaneous increase in the rate of disturbance inside the module, which explains a longer shoot response. However, a lower rate of disturbance occurs at the second step change, producing a lower shoot response after increasing the feed flow rate at a decent high feed flow rate.

It is clear from Figure 6.103 that increasing inlet pressure can increase the retentate concentration as a result of increasing the quantity of water flux. In this respect, the responses of the average permeate concentration and dimethylphenol rejection require a longer time to settle after implementing the second ramped change to attain the maximum feed flow rate tested at $7\text{E-}4 \text{ m}^3/\text{s}$ for a medium operating pressure of 10 atm (Figures 6.104 and 6.105). However, the response of both the average permeate concentration and solute rejection at 12 atm is comparable to the case of 10 atm. Interestingly, a noticeable decrease in dimethylphenol rejection at the operating

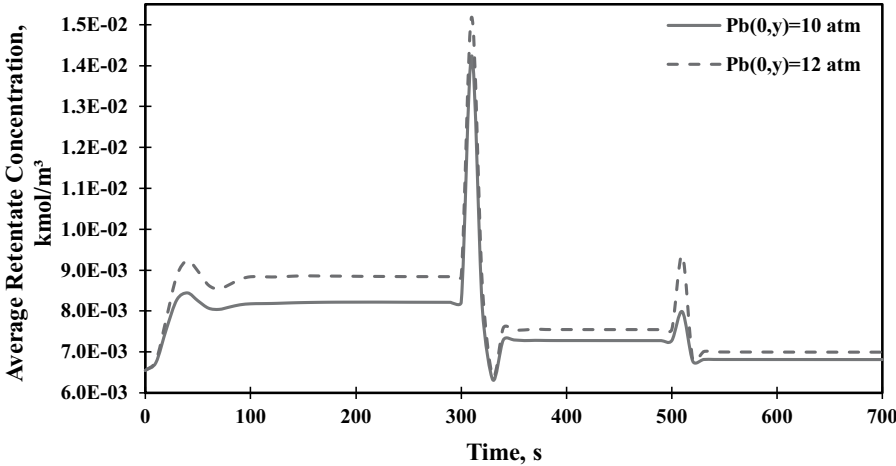


FIGURE 6.103 The result of the ramp change of feed flow rate on retentate concentration for operating conditions of $6.548 \times 10^{-3}\text{ kmol/m}^3$, $2.166 \times 10^{-4}\text{ m}^3/\text{s}$, 10 atm, and $31.5\text{ }^\circ\text{C}$.
(Adapted from Al-Obaidi et al., 2018b)

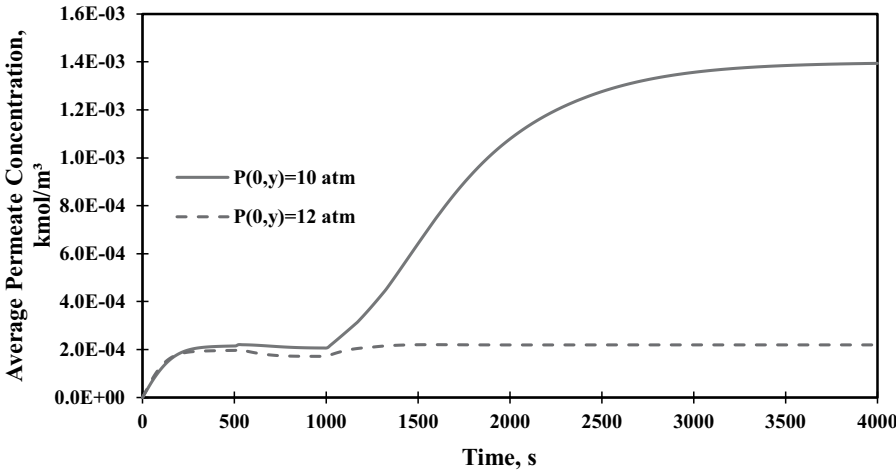


FIGURE 6.104 The result of the ramp change of feed flow rate on average permeate concentration for operating conditions of $6.548 \times 10^{-3}\text{ kmol/m}^3$, $2.166 \times 10^{-4}\text{ m}^3/\text{s}$, 10 atm, and $31.5\text{ }^\circ\text{C}$.
(Adapted from Al-Obaidi et al., 2018b)

pressure of 10 atm is achieved compared to a slight change at 12 atm. The explanation for this phenomenon is the fact that the combination of the high feed flow rate and the medium pressure of 10 atm was not sufficient for reducing the dimethylphenol rejection. However, the implementation of 12 atm has enhanced the dimethylphenol rejection and kept the rejection at a fixed value approximately.

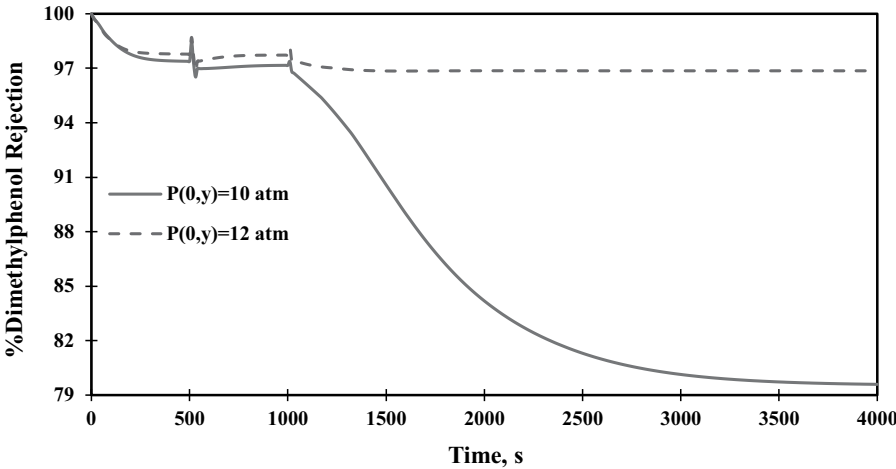


FIGURE 6.105 The result of the ramp change of feed flow rate on solute rejection for operating conditions of 6.548×10^{-3} kmol/m³, 2.166×10^{-4} m³/s, 10 atm, and 31.5 °C. (Adapted from Al-Obaidi et al., 2018b)

6.5.3.3 Inlet Feed Concentration

The dynamic impacts of a step change in inlet feed concentration on the average retentate concentration, average permeate concentration, and solute rejection for a set of inlet feed pressure at fixed inlet feed flow rate and temperature are given in Figures 6.106, 6.107, and 6.108 respectively. Figure 6.106 is conveniently drawn with different time axes compared with Figures 6.107 and 6.108 to show the impact of the step change on the given parameters. Specifically, the inlet feed concentration was $0.819\text{E-}3$ kmol/m³ up to $t = 1000$ s, and then it was increased to $6.548\text{E-}3$ kmol/m³ at $t = 1000$ s.

As predicted, increasing the inlet feed concentration causes an increase of the retentate concentration. This readily increases the average dimethylphenol concentration in the permeate channel due to a lower water flux.

Interestingly in this case, steady state conditions require more time compared with other step changes discussed earlier. This may be due to the degree of instability throughout the step change of the inlet feed concentration. The simulation results of a step change in the inlet feed concentration show that more time is required for the process to settle at low feed pressure conditions compared to high feed pressure ones (Figures 6.107 and 6.108). It is therefore fair to say that the use of a low operating pressure would generate a lower water flux. This would require more time for the dimethylphenol concentration at the permeate channel to get to the steady state compared to that observed for the higher pressure case. The use of higher feed pressure leads to higher water flux, thus allowing the permeate concentration to settle faster.

Figure 6.108 depicts the increase of dimethylphenol rejection due to an increasing operating concentration. It can also be seen in this figure that the consequence

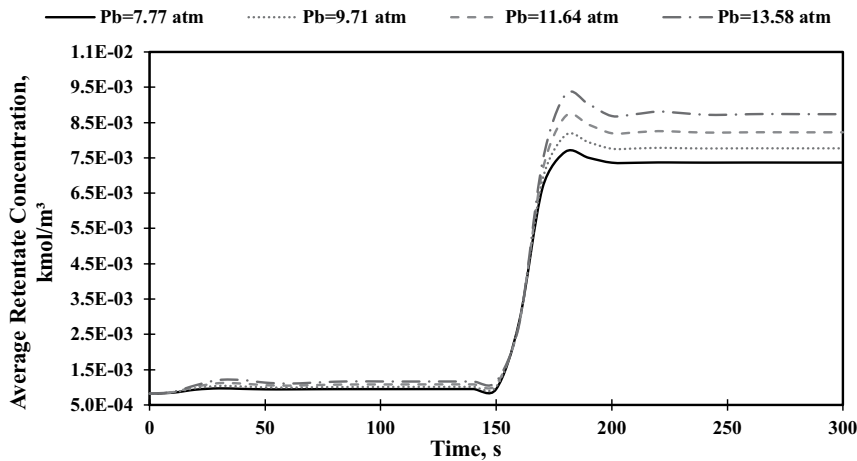


FIGURE 6.106 The result of the step change of operating concentration on retentate concentration for several operating pressures at operating conditions of $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, $0.819 \times 10^{-3} \text{ kmol/m}^3$, and $31.5 \text{ }^\circ\text{C}$.

(Adapted from Al-Obaidi et al., 2018b)

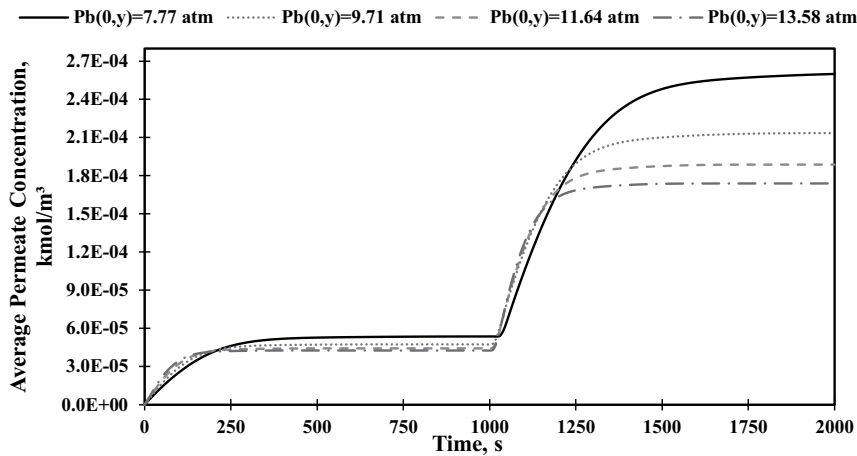


FIGURE 6.107 The result of the step change of operating concentration on average permeate concentration for several operating pressures at operating conditions of $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, $0.819 \times 10^{-3} \text{ kmol/m}^3$, and $31.5 \text{ }^\circ\text{C}$.

(Adapted from Al-Obaidi et al., 2018b)

of a step change in the feed concentration results in a significant overshoot in the rejection. This may be the result of increasing the concentration on the feed channel, as more specifically shown in Figure 6.106. Here again, the improvement of dimethylphenol rejection is clearly related to the use of higher operating pressures (Figure 6.108) compared to lower ones.

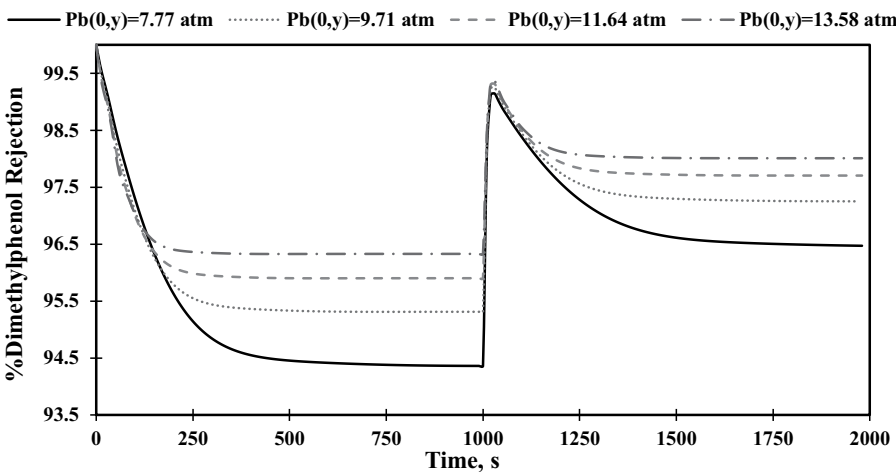


FIGURE 6.108 The result of the step change of operating concentration on rejection parameter for several operating pressures at operating conditions of 2.583×10^{-4} m³/s, 0.819×10^{-3} kmol/m³, and 31.5 °C.

(Adapted from Al-Obaidi et al., 2018b)

6.5.3.4 Inlet Feed Temperature

The dynamic impacts of a step change in inlet feed temperature on the average retentate concentration, average permeate concentration, and solute rejection respectively for a set of inlet feed pressures at fixed inlet feed flow rate and concentration are given in Figures 6.109 to 6.111, respectively. Figure 6.109 is conveniently drawn with different time axes compared with Figures 6.110 and 6.111 to show the impact of the step change on the given parameters. Specifically, the inlet feed temperature was 31.5 °C up to $t = 1000$ s, and then increased to 40 °C at $t = 1000$ s.

The retentate concentration of dimethylphenol profile to a step change in the operating temperature can be seen in Figure 6.109. It is clear that increasing the temperature decreases the viscosity and density parameters and lifts up the permeation of water, which then causes an increase of the retentate concentration. However, it seems that the process requires a longer time to settle when a step change in the temperature is carried out. Additionally, increasing the operating temperature causes a clear reduction of the average permeate concentration (Figure 6.110) and increases the dimethylphenol rejection (Figure 6.111). Whilst these results are in line with those of Mohammadi et al. (2009) for the removal of chromium from wastewater, they are somewhat different than those of Fujioka et al. (2014) for the removal of N-nitrosamine from wastewater. The size exclusion (low molecular weight of N-nitrosamine) might interpret the reason behind this. Interestingly, the underdamped response without clear overshoots before reaching the steady state appears to be typical for the average retentate concentration, average permeate concentration, and the solute rejection towards a step change in the operating temperature. This is specifically compared to the other tested cases of step change in operating pressure, concentration, and flow rate. Nevertheless, the same behaviour has also been

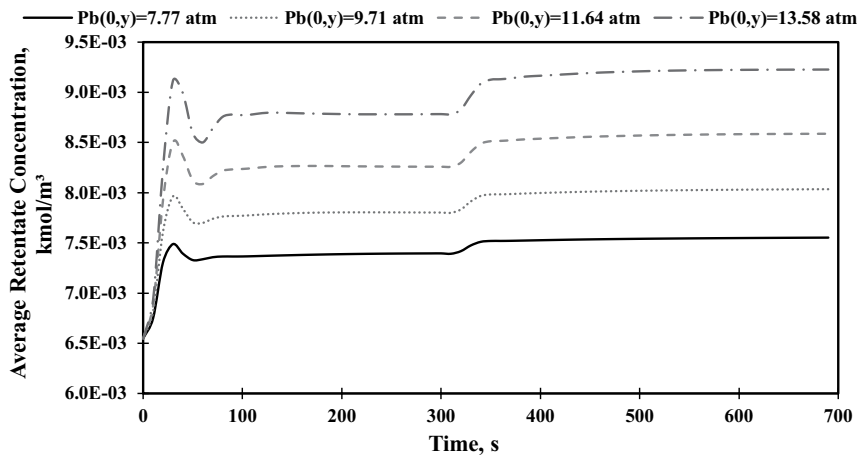


FIGURE 6.109 The result the step change of operating temperature on retentate concentration for several operating pressures at operating conditions of $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, $6.548 \times 10^{-3} \text{ kmol/m}^3$, and 31.5°C .

(Adapted from Al-Obaidi et al., 2018b)

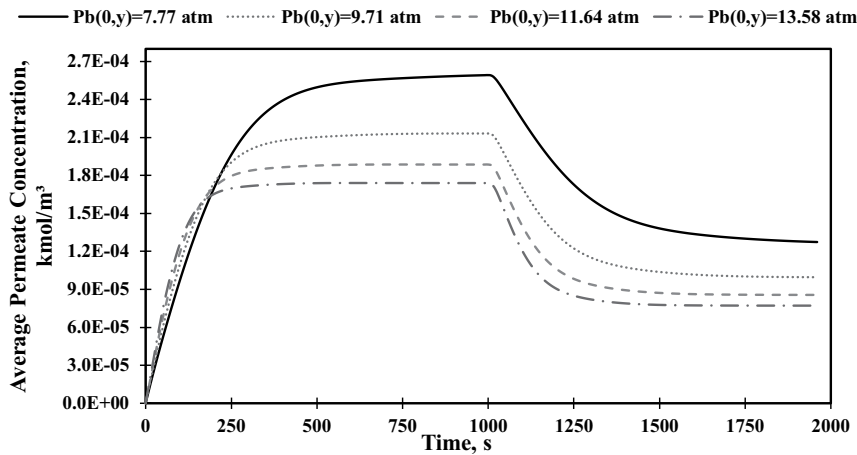


FIGURE 6.110 The effects of the step change in operating temperature to mean permeate concentration for several operating pressures at operating conditions of $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, $6.548 \times 10^{-3} \text{ kmol/m}^3$, and 31.5°C .

(Adapted from Al-Obaidi et al., 2018b)

observed for average permeate concentration after imposing the step change of pressure, concentration, and flow rate. This can be attributed to the lower degree of disturbance that can occur in the medium after imposing a step change of temperature from 31.5°C to 40°C , compared to a higher degree of disturbance that is expected to occur at other step changes of operating parameters.

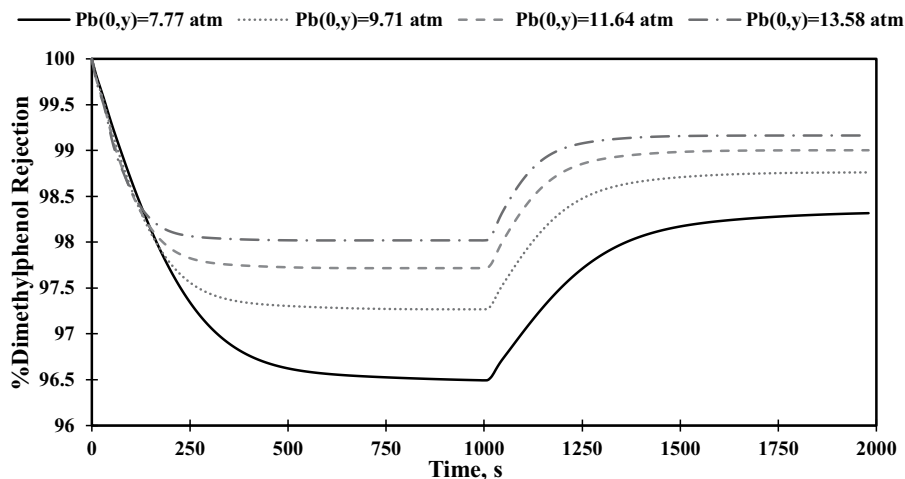


FIGURE 6.111 The result of the step change of operating temperature on rejection parameter for several operating pressures at operating conditions of $2.583 \times 10^{-4} \text{ m}^3/\text{s}$, $6.548 \times 10^{-3} \text{ kmol}/\text{m}^3$, and 31.5°C .

(Adapted from Al-Obaidi et al., 2018b)

6.6 CONCLUSIONS

This chapter has reviewed and discussed several case studies of steady state and dynamic simulations to elucidate the transport phenomena of RO processes for the removal of several harmful pollutants from wastewater. The simulation studies discussed are based on experimentally validated RO process models, which have been developed for the removal of pollutants from wastewater (Chapter 5). The impact of several operating conditions on process performance have been thoroughly analysed under steady state and dynamic operation.

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7 Optimisation of RO Process Superstructure for Wastewater Treatment

7.1 INTRODUCTION

The need for desalinated seawater and reclaimed wastewater is increasingly becoming critical for an ever-growing world population requiring higher demands for fresh water. At the same time, there has been an equal rising demand for more energy resources and stricter environmental protocols. The discharge of wastewater without proper treatment is no longer acceptable as it has a major impact on humans and the ecosystem. The reuse of treated wastewater continues to be the most feasible and economical solution not just for the industrialised world but also for several developing countries. Nowadays, many countries around the world have a wide experience in increasing freshwater supply by treating wastewater and reclaiming water, and they have achieved this at reasonable costs and in line with environmental legislation (Bixio et al., 2006). Many such applications around the world have focused on the reverse osmosis (RO) process as it offers an efficient economic separation process at a lower energy demand compared with thermal processes such as multi-stage flash (MSF) and multi-effect distillation (MED). Indeed, the RO process is now among the most promising technologies used to efficiently remove organic and non-organic compounds from industrial wastewater of several industries (Chapters 4, 5, and 6). Such removal efficiency, however, does not readily include low molecular organic compounds such as N-nitrosamine. An improved RO process performance is therefore required. Several attempts for achieving this have focused on optimising the process network and operating conditions in order to minimise costs and maximise solute rejections at an acceptable energy consumption. Many such attempts have resulted in the determination of the optimal settings for the conditions and networks.

The performance of an RO process is very sensitive to many aspects, including module arrangements, size, number, type, and more importantly, the operating conditions of feed flow rate, applied pressure, concentration, and operating temperature. These factors have a major impact on the removal rate of micropollutants and the associated energy requirements, which serve to minimise the cost of water production.

In this chapter, several process optimisation methodologies are reviewed and their principles discussed. Examples of the most successful superstructure optimisation

of RO networks, for wastewater treatment used for the removal of high toxic compounds, are described in detail.

7.2 PROCESS OPTIMISATION: PROBLEM FORMULATION

Optimisation is generally used to identify and select the most effective solution for a given process. This is achieved by optimising one or more operating variables in order to reach a specific objective. As such, optimisation problems may entail maximising or minimising selected objective functions under consideration and relying on several typical constraints. The combination of process modelling, simulation, and optimisation can be used to produce desired systems at low costs. Several authors have discussed this in more detail, and they include Mujtaba (2004), Hendrix and Tóth (2010), Horst and Tuy (2010), and Eiselt and Sandblom (2010).

A simple formulation of any optimisation problem can be mathematically represented as: (Mujtaba, 2004 and El-Halwagi, 2006);

Max or Min

$f_{(x_1, x_2, \dots, x_n)}$

$f_{(x_1, x_2, \dots, x_n)}$ denotes the objective function and in $(x_1, x_2, \dots, x_n)$, n denotes the decision variables which need to be optimised to attain the objective function and the number of decision variables, respectively. The objective function must quantify the equality constraints as:

Equality constraints:

$f(x_1, x_2, \dots, x_n) = 0$

Also, the objective function must satisfy the inequality constraints of the process, which can be specified as equal, less than, or more than zero. For example:

Inequality constraints:

$g_1(x_1, x_2, \dots, x_n) \leq 0$

$g_2(x_1, x_2, \dots, x_n) \leq 0$

$g_n(x_1, x_2, \dots, x_n) \leq 0$

Simply, the objective function of any optimisation problem that contains non-linear constraints is called non-linear programming (NLP). Otherwise, if the constraints are linear, the optimisation problem is called linear programming (LP). A mixed integer non-linear programming (MINLP) problem refers to an optimisation problem that contains non-linear continuous real variables such as pressure or temperature and binary integer variables. An MINLP solution was used to (a) synthesise cost-effective mass-exchange networks which were initially innovated by El-Halwagi and Manousiouthakis (1989), (b) synthesise multi-stage flash desalination process by Tanvir and Mujtab (2008), and (c) synthesise RO desalination process by Sassi and Mujtaba (2013).

Several steps are required to formulate the optimisation problem recommended by El-Halwagi (2006). They are as follows:

- Understand the main concepts of the process and determine the rationale for optimising one or several process parameters given their constraints.
- Improve the clarity of the process model. This basically means the necessity of providing an accurate mathematical model that is able to capture the core of the problem.
- Specify the objective function: this includes the determination of a specific objective function and the decision variables that need to be addressed in their lower and upper bounds.
- Determine the equality and inequality constraints: this would include the restrictions of the process and their mathematical description. It is important to have enough standpoints to generate useful bounds of these continuous variables. Also, it is recommended to prevent the use of highly non-linear constraints that might cause some difficulty in attaining reasonable solutions.
- Use an appropriate mathematical software to find effective solutions and to carry out sensitivity analysis.

The RO superstructure optimisation is an effective tool that can be used for determining a feasible distribution of units and module configurations within a given network, as well as providing an optimal operation of each module.

The RO network superstructure optimisation has several merits and they include (Khor et al., 2011):

- It can manage large-scale complex RO network systems.
- It is an efficient tool for minimising the associated cost functions.
- It can handle several contaminants.
- It can consider a wide range of topological constraints.

7.3 SOLUTION OF RO OPTIMISATION PROBLEMS

Several case studies relating to the optimisation of RO process performance can be found in the open literature. These include the investigation of the transport phenomena of water and solute through the membrane using improved mathematical models and identifying the optimum set of operating variables. The main aim of an RO process optimisation is to identify the best design and operating parameters, which can yield the maximum process performance at minimum energy consumption and within the manufacturer's specification. Water production costs as well as requirements of zero discharge pollutants (as in many countries) can readily be incorporated in the optimisation problem. Many optimisation methodologies and mathematical programming (constrained optimisation) are used in practice. These include Lagrange multipliers, linear and non-linear programming, dynamic programming, quadratic programming, fractional programming, and geometric programming (Loucks and Beek, 2017). The selection of a suitable solution method is basically dependent on the process structural model. Several attempts can be found in the

literature where a non-linear programming methodology has been used to optimise the RO process. These include successive linear programming (SLP) and sequential quadratic programming (SQP) (Villafafila and Mujtaba, 2003), global optimisation algorithm (GOP) (Marcovecchio et al., 2005), genetic algorithm (GA) (Murthy and Vengal, 2006) and multi-objective optimisation and genetic algorithm (MOO+GA) (Guria et al., 2005). Also, Lu et al. (2006) used a complex NLP of mixed integer non-linear programming methodology. Sassi and Mujtaba (2013) used MINLP in a model for the removal of boron from seawater using an RO process. The remainder of this book demonstrates applications of the most commonly used NLP and GA methodologies in the optimisation of an RO process for wastewater treatment. To this extent, the superstructure optimisation using MINLP methodology is provided briefly. The next sections of this chapter discuss in detail the principles of the NLP solution methodology as applied to the superstructure optimisation problem at hand. The next chapter concentrates more on the GA optimisation methodology as applied to an RO process in wastewater treatment.

7.3.1 NLP-BASED OPTIMISATION

There are several software suites that can be used to solve optimisation problems, such as LINGO developed by LINDO Systems Inc. (<https://www.lindo.com/>) and gPROMS (general Process Modelling System) Model Builder developed by Process System Enterprise Ltd. (2001). These software suites can be used to solve several types of optimisation problems including linear, non-linear, and mixed integer linear and non-linear programs. gPROMS can solve steady state optimisation problems (point optimisation entities) of non-linear programming problems. Point optimisation technique (POT) is mathematically equivalent to solving a purely algebraic problem without the consideration of maximising or minimising a non-linear objective function subjected to general non-linear constraints (equality and inequality constraints) of upper and lower limits of operation. The solution of this optimisation problem is carried out by manipulating a set of optimisation decision variables, which for example may characterise pressure or temperature, that may be either continuous or discrete. This provides a prediction of the appropriate operating conditions which yield the objective function. gPROMS includes an option for the sequential quadratic programming technique which is used to solve NLP problems, as described more particularly in the next section.

7.3.1.1 Successive Quadratic Programming technique

The sequential quadratic programming (SQP) method can be used to solve steady state optimisation problems (point optimisation entities) and dynamic optimisation by implementing a first-order Taylor's series approximation around an initial point specified in the process. This converts the non-linear functions into approximate linear functions. In other words, the process prepares the optimisation by converging all the equality constraints (including the model equations) and inequality constraints. Secondly, the optimisation step starts by updating (re-initialising) the values of the decision variables (Edgar et al. 2001). This locates a new search direction for the decision variables, which is achieved using the solution of the last successful iteration. The new values of the decision variables become the initial point (guestimate

values) required to solve the linear problem. This is continued until a solution of the linear problem with a specific improvement of the objective function is obtained. One of the standard solvers in the gPROMS software for optimisation problems is CVP_SS, which uses the DASOLV code for this purpose. This can be used to solve steady state and dynamic optimisation problems with both discrete and continuous optimisation decision variables (mixed integer optimisation).

7.3.2 SUPERSTRUCTURE OPTIMISATION

Rigorous wastewater discharge standards, with a wide-range of chemicals and high-toxic pollutants, has motivated process designers and decision-makers to seek highly effective designs based on optimisation. RO is a pressure-driven process, which has been applied in a growing number of applications in the field of high-toxicity mitigation. An RO network is the same as other chemical processing plants, in that it contains several units linked in series, parallel and recycle streams. The main idea of superstructure optimisation and synthesis of a RO network is simply based on minimising the wastewater treatment cost by converting the feed streams into product streams and retentate streams in an optimal network of RO modules, pumps, and ERDs. More importantly, it is necessary to achieve this treatment within environmental and operational constraints and regulations. In other words, the superstructure optimisation would effectively be based on the input and output information to map the objective function by designing the best route to adjust the feed streams into product streams. The idea was initially used by El-Halwagi (1992) to generate a product and retentate streams using an efficient RO network of multiple units.

The RO process synthesis is mainly governed by economic and environmental aspects in addition to other process constraints (Grossmann, 2004). The RO superstructure method can be used to find the most feasible design which can attain the lowest total annualised cost and energy consumption. Fundamentally, TAC (total annualized cost) comprises the costs of pumps, ERDs (used to recover kinetic energy from retentate high-pressure stream), and RO units and operational costs such as power consumption and membrane replacement. Therefore, the optimal solution of RO network leads to the optimal arrangements, types, and size of RO units, pumps, and ERDs. Moreover, the effective operating conditions, stream distribution, and separation levels are also achieved through superstructure optimisation.

The superstructure optimisation methodology contains several challenges that need to be tackled before designing the RO networks. These challenges are as follows:

- The complexity of selecting the optimal arrangement of multiple units of RO system from different connecting methods. This include series, parallel, and hybrid arrangements.
- The operating conditions of each unit with signifying its size, type, and number should be taken into consideration.
- The inclusion of pumps, booster pumps, and ERDs are important for any RO network. There is a clear complexity of the selection of their efficiency, size, and locations.

- The distributions of the product and retentate streams and their connection, by-pass, and recycle streams are important for optimisation.
- The wastewater of several applications contains a wide range of hazardous chemicals with different specifications. This would add another challenge to professionally design the RO network to maintain a simultaneous and effective removal of those pollutants.

El-Halwagi (1992) used the state-space methodology of El-Halwagi (1989) to synthesise the RO network. This approach serves the consideration of all possible connections between the units and outlet and inlet network streams. The proposed method basically relies on the nonconvexity of the mathematical program (MINLP). It is therefore fair to expect several local superstructure solutions as well as a global solution. The state-space approach optimisation method can be considered as an effective tool for incorporating several RO networks, one of them being the optimal layout.

Figure 7.1 shows a generic superstructure of any synthesised network problem as adopted by El-Halwagi (1992). This includes a large distribution box (DB) that encompasses several entering and leaving streams and that mixes or splits streams before and after the unit operations. *WI* and *USI* are a set of inlet wastewater streams and utility streams used to achieve a specific task, respectively. *WO*, *P*, and *USO* are a set of outlet wastewater streams, a set of product streams, and a set of utility streams departing the RO network, respectively. *UO* and *O* denote a set of utility unit operations and a set of unit operations, respectively.

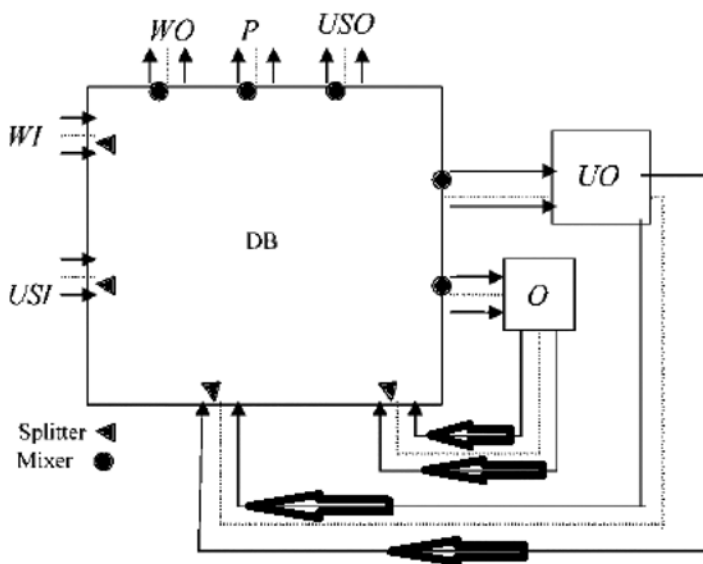


FIGURE 7.1 Generic superstructure presentation of any synthesized network problem.

(Adapted from Saif et al., 2009)

The optimisation problem can therefore be formulated to maximise or minimise an objective function under equality and inequality constraints. Moreover, it combines several parameters and continuous and discrete variables. A simple mathematical representation of a superstructure optimisation is shown as follows:

$$\begin{array}{ll} \text{Objective function:} & \text{Max or Min} \quad f(x,y) \\ \text{Subject to:} & h(x) = 0 \\ & g(x) + My \leq 0 \end{array}$$

$f(x,y)$ is the objective function to be minimised or maximised. x , y are vectors of continuous and binary variables. Continuous variables denote concentration, flow rate, and pressure, while binary variables denote the existence of units or streams. $h(x)$ denotes the equality constraints that refer to unit models. However, the inequality constraints depict the relationship between the continuous and binary variables.

7.4 OVERVIEW OF THE SUPERSTRUCTURE OPTIMISATION FOR AN RO PROCESSES-BASED WASTEWATER TREATMENT

Multistage RO stages are basically connected in several networks using pumps and ERDs. The optimisation of such an RO process for wastewater treatment and the use of a superstructure synthesis has been addressed by several authors. In this respect, the optimal layout of the RO process, including high-pressure pumps, ERDs, and RO stages, can be achieved by formulating the problem as an MINLP optimisation problem.

Many researchers used RO network synthesis problems for minimising the water consumption and the total annualised cost of the wastewater treatment.

El-Halwagi (1992) investigated the optimal RO network for the removal of two organic chlorophenolic compounds from wastewater of the pulp production industry. The state-space optimisation framework was adopted for structural representation by considering continuous and discrete variables to minimise the total annualised cost. This provided the estimation of the operational conditions, connected streams, and separation levels within the operational and environmental constraints.

The same optimisation framework of nonconvex MINLP methodology was used by El-Halwagi (1993) for synthesising an optimal network for the hybrid system of regeneration units, mass exchangers, RO modules, booster pumps, and ERDs. This has shown the possibility of minimising TAC to US\$6,811,948 per year for the hybrid system of two stages of RO process, pump, ERD, adsorption and desorption columns, and the extraction column.

Saif et al. (2008) enhanced the RO network of Halwagi (1993) by formulating the MINLP nonconvex problem as a mixed-integer linear problem (MILP). This resulted in more feasible connections between the RO units. An optimal RO network for the removal of two chlorophenolic compounds from pulp wastewater at minimum total annualised cost was obtained.

Khor et al. (2011) presented extensive research which helped minimise the water consumption and total annualised cost of an existing oil refinery plant. This was

carried out by embedding an RO network into a water network and investigating a feasible flowsheet of the overall network based on the state-space approach of MINLP optimisation framework. This study confirmed a substantial reduction of water consumption of 58% compared to the existing water network.

Saif et al. (2013) built an optimisation framework based on a state-space approach to minimise the water consumption and total treatment cost of the pulp and paper industry. The suggested water recycle and reuse with the addition of a regeneration RO unit had a significant impact on attaining the main objective optimisation functions. The projected pollutant was NaCl, which was efficiently minimised as a result of this optimisation. A reduction of 13% of freshwater consumption and a high performance of NaCl removal were observed in this study.

Buabeng-Baidoo and Majozi (2015) improved the work of Khor et al. (2011) by optimising the water network and investigated other opportunities and scenarios of adding RO regeneration units to the original water network. This helped explore a high-efficient-energy layout, which can simultaneously treat multiple pollutants. More importantly, this study showed that implementing the variable removal ratio of contaminants yields a reduction of 28% in the freshwater consumption compared to the original water network. This corresponds to a considerable reduction of 80% of wastewater generation.

Abass and Majozi (2016) tested the opportunity of synthesising a high-efficient regeneration water network instead of the original water network of an existing pulp and paper industry. This was based on adding electrodialysis (ED) and hollow fibre RO processes into the water network and optimising the overall network to attain the lowest treatment cost from several proposed scenarios. The global solution affirmed the possibility of reducing the freshwater consumption and wastewater generation by 43.7% and 50.9%, respectively.

Buabeng-Baidoo et al. (2017) assessed the viability of using an RO generation unit in an original water network of a dairy plant to reduce the freshwater consumption used in cleaning, treatment cost, and wastewater generation. They used an MINLP optimisation framework to achieve the nominated objective functions. The membrane characteristics, operating conditions, and a set of environmental and operational constraints were considered in the optimisation approach. This confirmed the opportunity of attaining a global solution for the overall water network that can mitigate the freshwater consumption, wastewater generation, and total annualised cost by 33%, 85%, and 33%, respectively.

Al-Obaidi et al. (2018) carried out a comprehensive single objective optimisation problem to select an optimum layout (amongst many) of multistage RO process for the maximum removal of dimethylphenol from wastewater. This confirmed that a parallel layout can attain the highest removal of dimethylphenol and at the same time fulfil the recommended instructions of the membrane's manufacturer.

7.5 OPTIMAL RO NETWORK FOR THE REMOVAL OF TWO CHLOROPHENOLIC COMPOUNDS FROM PULP WASTEWATER

The production of wood pulp can be considered as the main process in the paper industry. This industry finishes the washing up of chlorinated pulp using water and filtration units. The produced wastewater contains two highly toxic chlorophenolic compounds of monochlorophenol (MCP) and trichlorophenol (TCP). El-Halwagi

(1992) investigated an optimal RO network, pumps, and ERDs for waste-reduction applications based on multiple RO modules. This was used to separate MCP and TCP compounds from wastewater. The optimal network has taken into consideration all the RO system compounds and their interactions and stream distributions. Interestingly, the optimisation used the minimisation of the total annualised cost (TAC) of the RO network as the objective function. The TAC satisfies the annual operating cost and annualised investment cost. More specifically, the optimisation has considered a number of binary integer variables, which signify the use or non-use of RO, pumps, and ERD units. Several technical and environmental constraints were imposed in this study. Specifically, the environmental regulations of these chlorophenolic compounds were set as the discharged concentrations. Also, the operating conditions of each RO unit (type: Du Pont B-9 modules) were considered, which included the flow rate and concentrations of the characteristics of rejected and product streams of each nominated stage. Furthermore, the characteristics of each module with their upper and lower operating constraints were included. Figure 7.2 shows

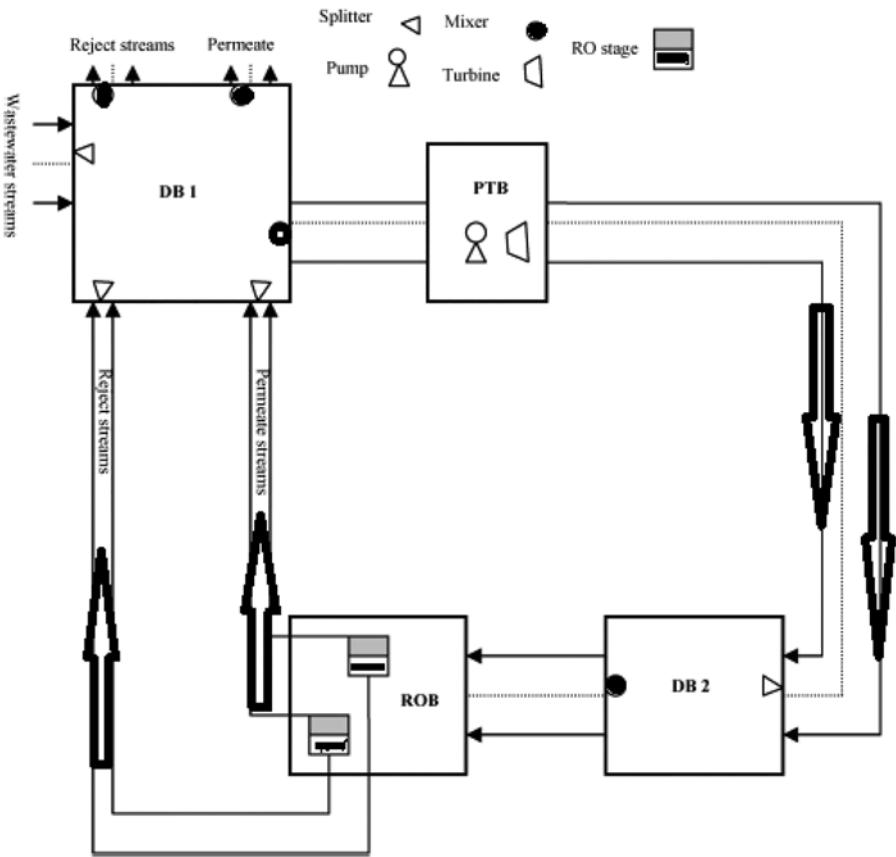


FIGURE 7.2 Integrated RO superstructure representation of El-Halwagi (1992).

(Adapted from Saif et al., 2009)

a number of unit operations in the RO superstructure representation as developed by El-Halwagi (1992). It contains two distribution boxes (DB1 and DB2), a pump-turbine box (PTB), and an ROB (RO stage box). The wastewater streams leave DB1 and enter PTB to be pressurised or depressurised and are then directed to DB2 to be delivered afterwards to ROB. The possibility of stream bypassing is considered due to blending the outlet streams of ROB with the inlet streams of wastewater. Table 7.1 shows the input data for the optimisation. The global optimal solution of the RO network for the removal of MCP and TCP is depicted in Figure 7.3, which shows three RO stages of 77 modules, two pumps, and two ERDs. The data on each stream as given in Figure 7.3 show the mass flow rate, mass fraction of MCP and TCP, and pressure. The optimisation resulted in a minimum total annualised cost of \$193,420 per year, which has yielded a more efficient and environmentally friendly RO process.

TABLE 7.1
Input Data for the MINLP Optimisation Problem

Variable	Value
Feed flow rate of the first waste stream kg/s	6.0
Feed flow rate of the second waste stream kg/s	25.0
Feed concentration of MCP in the first waste stream	26×10^{-6}
Feed concentration of TCP in the first waste stream	3×10^{-6}
Feed concentration of MCP in the second waste stream	12×10^{-6}
Feed concentration of TCP in the second waste stream	4×10^{-6}
Max. of acceptable flow rate of permeate for the first waste stream kg/s	4.5
Max. of acceptable flow rate of permeate for the second waste stream kg/s	9.0
Max. allowed concentration of MCP in the permeate of the first waste stream	8.8×10^{-6}
Max. allowed concentration of TCP in the permeate of the first waste stream	1.4×10^{-6}
Max. allowed concentration of MCP in the permeate of the second waste stream	8.8×10^{-6}
Max. allowed concentration of TCP in the permeate of the second waste stream	1.4×10^{-6}
Max. and Min. flow rates for each module kg/s	0.46 and 0.21
Max. feed pressure N/m ²	25.58×10^5
Pressure drop of each module N/m ²	0.405×10^5
Water permeability kg/s N	1.2×10^{-10}
MCP solute transport parameter kg/m ² s	2.43×10^{-4}
TCP solute transport parameter kg/m ² s	2.78×10^{-4}

(Adapted from El-Halwagi, 1992)

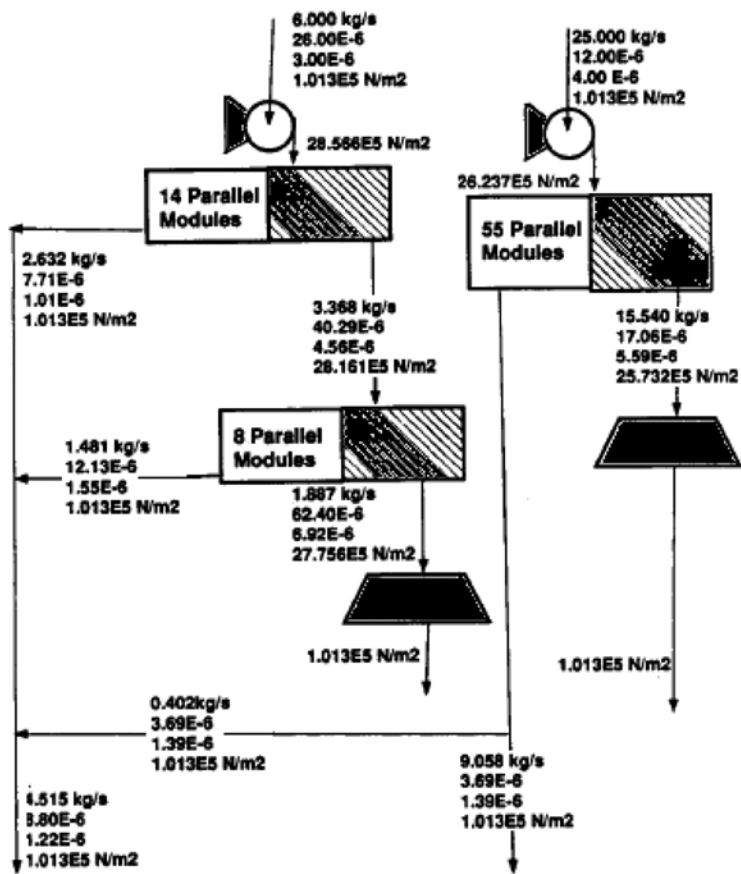


FIGURE 7.3 Optimal RO network for the removal of MCP and TCP.

(Adapted from El-Halwagi, 1992)

7.6 OPTIMAL RO NETWORK FOR THE REMOVAL OF PHENOL FROM WASTEWATER OF LUBE-OIL RECYCLING PLANTS

The RO process is one of the most effective separation methods which has been used for the removal of phenol from oily wastewater. The integration of an RO process with other mass-exchange processes can produce an improved separation performance. El-Halwagi (1993) investigated the optimal network using a state-space approach for the hybrid system of RO unit (type: Du Pont B-9 modules) and mass exchanger units. These include extraction, adsorption, and desorption columns. Phenol is used as an oxidation inhibitor to mitigate sediment formation and enhance colour stability. The optimisation is based on minimising the total annualised cost while satisfying several technical and flexible constraints. Input data of the optimisation problem are

TABLE 7.2
Input Data for the MINLP Optimisation Problem

Variable	Value
Feed flow rate (phenol free) kg/s	131.42
Feed phenol concentration	4×10^{-3}
Max. of acceptable flow rate of permeate kg/s	131.42
Max. allowed concentration of phenol in the permeate	0.04×10^{-3}
Max. and Min. flow rates for each module kg/s	0.46 and 0.21
Max. feed pressure N/m ²	25.58×10^5
Pressure drop of each module N/m ²	0.405×10^5
Water permeability kg/s N	1.2×10^{-10}
Phenol solute transport parameter kg/m ² s	2.43×10^{-4}

(Adapted from El-Halwagi, 1993)

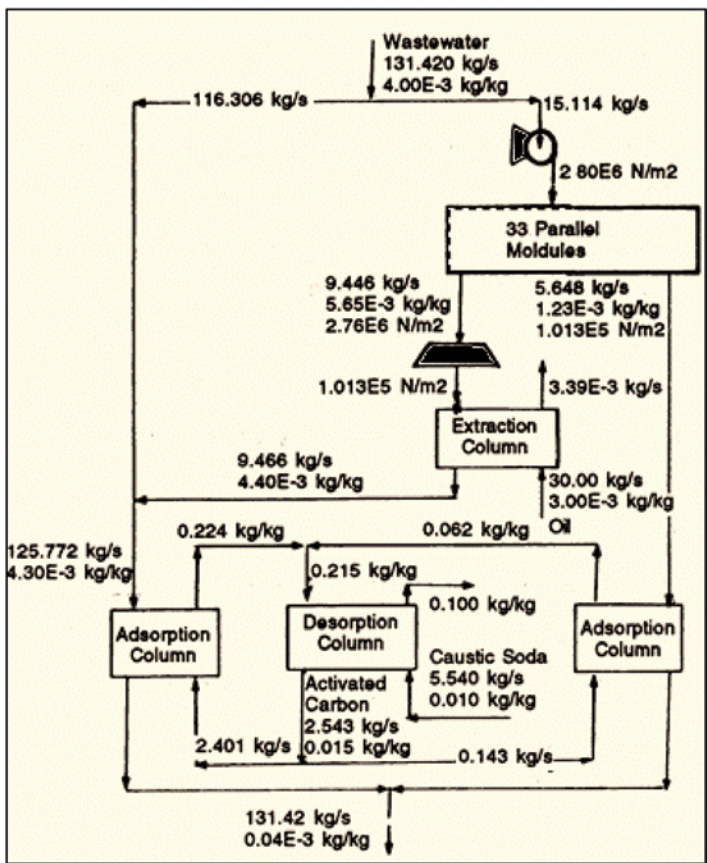


FIGURE 7.4 Optimal RO network for the removal of phenol from oily wastewater.

(Adapted from El-Halwagi, 1993)

presented in Table 7.2. The solution of an optimal hybrid system network using the MINLP algorithm is shown in Figure 7.4. The proposed solution specifies the use of one extraction column, one adsorption column, one desorption column (regeneration unit), one pump, one ERD, and 33 modules of two stages of RO process resulting in a minimum cost of \$6,811,948 per year.

7.7 OPTIMAL RO NETWORK FOR THE REMOVAL OF TWO CHLOROPHENOLIC COMPOUNDS FROM PULP WASTEWATER USING AN ADVANCED OPTIMISATION METHOD

The MINLP optimisation of any RO network has non-linearities and non-convexities as a result of bilinear terms. Saif et al. (2008) modified the superstructure given by Halwagi (1993) by developing an advanced optimisation method of RO network for water and wastewater treatment. The improved method is essentially based on the discretisation of one of the variables of the bilinear terms. Saif et al. (2008) made an exclusion of several alternatives among the utility pumps and ERD units and the addition of other alternatives in the RO network. This simplifies the modelling of the RO network considered by Halwagi (1993) and offers plausible connections between the RO units. More specifically, the RO network optimisation problem was initially formulated as an MINLP nonconvex problem and then formulated as a mixed-integer linear problem (MILP) as a result of relaxing the nonconvex terms in the MINLP

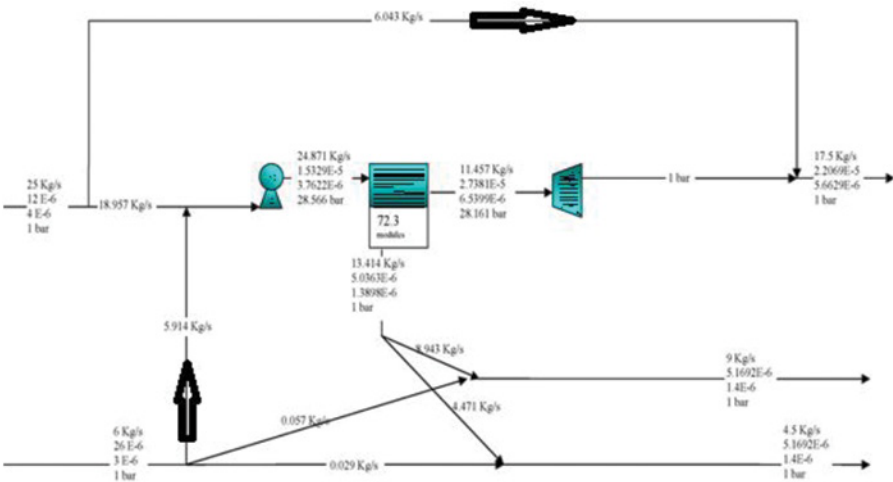


FIGURE 7.5 Optimal RO network for the removal of MCP and TCP in pulp wastewater treatment.

(Adapted from Saif et al., 2008)

methodology, which deliver a specific lower bound for the global solution. In other words, a wide range of initial guesstimates for the MINLP model was provided due to solving the associated MILP model in an iteration (multi-start search method). This led to an effective global RO network solution.

The modified optimisation framework was tested on wastewater with monochlorophenol and trichlorophenol pollutants considered earlier by El-Halwagi (1992) with the objective of minimising total annualised cost. Input data for the optimisation problem are already presented in Table 7.2. The global optimisation showed \$152,406/year of TAC with a superstructure containing three stages of RO process, three pumps, and three ERDs as shown in Figure 7.5. One of the important observations of the proposed global network is the advantages of partial mixing of the feed wastewater streams, which results in the reduction of TAC compared to that obtained by El-Halwagi (1992).

7.8 MINIMISATION OF FRESHWATER INTAKE IN A PETROLEUM REFINERY

Khor et al. (2011) studied the opportunity of minimising water consumption in a water network by adding a water regeneration unit for an operating oil refinery in Malaysia. The optimisation methodology suggested relied on a mechanistic model of the RO network developed earlier by El-Halwagi (1992 and 1997). The adopted model is embedded in an MINLP optimisation framework to solve an optimal regeneration network and minimise the total annualised cost. The optimisation problem considered several parameters described as follows:

- The inlet and outlet flow rates.
- The inlet and outlet concentrations.
- The membrane type and size.
- The arrangement of membrane modules.
- The optimal operating conditions.
- The type, size, and number of pumps and ERDs.

The upper and lower bounds of the continuous variables were considered in the MINLP methodology. They include the total feed flow rate, operating pressure, and osmotic pressure of retentate stream (referring to contaminant concentration). Binary variables (0, 1) are used to specify the existence of a stream piping interconnection. The non-linearity of MINLP is due to the existence of non-linear functions including bilinear terms in the regeneration unit (membrane unit), exponential terms, and power terms in the objective function. This optimisation resulted in multiple solutions of the RO network. The global solution of this nonconvex MINLP methodology is shown in Table 7.3 and consists of 20 RO membrane modules with an effective membrane area of 3780 m², giving the lowest total annualised cost (investment and operating costs) of \$96,291/year. However, the total annualised cost for the whole water regeneration network was \$2,738,000/year, which amounts to 58% savings in freshwater use compared to that of the original industrial operations.

TABLE 7.3
Optimisation Results

Parameter	Value
Total annualised cost of RO network	\$96,291/year
Total annualised cost of overall water regeneration network	\$2,738,000/year
Total freshwater use without water regeneration	705 ton/h
Total freshwater use with water regeneration	295.9 ton/h
Percentage of fresh water saving	58%
Number of RO network modules	20

(Adapted from Khor et al., 2011)

7.9 MINIMISATION OF FRESHWATER INTAKE OF PULP AND PAPER PROCESSES BY RECYCLING AND REGENERATION OF WASTEWATER STREAMS

Large quantities of water are consumed in several industrial applications, including pulp and paper manufacturing. The main pollutant is NaCl, which is very harmful to the ecosystem. Saif et al. (2013) evaluated the opportunities for minimising freshwater usage within pulp and paper processes by considering the recycling and regeneration of wastewater. This was achieved via a superstructure optimisation of an RO network allowing recycling of wastewater streams at a minimum cost and NaCl concentration.

Several parameters were considered for the optimisation, such as the number of RO stages, membrane surface area, and pump and ERD design and operation. The total annualised cost included both fixed and operating costs. The fixed costs included the RO modules, pumps, and ERDs. The operating costs included energy and membrane replacement costs. Additionally, the MINLP algorithm included several environmental and operational constraints.

A hollow fibre RO membrane was used in this study, and the specifications are reported in Table 7.4. The MINLP optimisation problem is illustrated in Figure 7.6. The optimal configuration is in fact three RO process modules with two high-pressure pumps and two ERDs. The retentate and permeate of the first module are treated further in modules 2 and 3, respectively. The optimal network design was able to increase the purity of the product as well as concentrating the retentate stream. The first pump can deliver the required energy to treat wastewater in the first module. However, the second pump can raise the operating pressure of feed forwarded to module 3. Two ERDs are used to extract energy from the high-concentration high-pressure retentates of modules 2 and 3. The total water recovery of the RO network is found to be 30%, and this is recycled back to the pulp and paper process. Interestingly, this accounts for a reduction of around 13% (7700 tons/day) of freshwater consumption and encompasses 98% and 97% removal of NaCl and KCl, respectively.

TABLE 7.4
Membrane Specifications

Module property	Unit	Value
Fibre length	m	0.75
Fibre seal length	m	0.075
Inner radius	M	21×10^{-6}
Outer radius	m	50×10^{-6}
Membrane surface area	m ²	152
Membrane type: Du Pont, B-10 Hollow Fibres		

(Adapted from Saif et al., 2013)

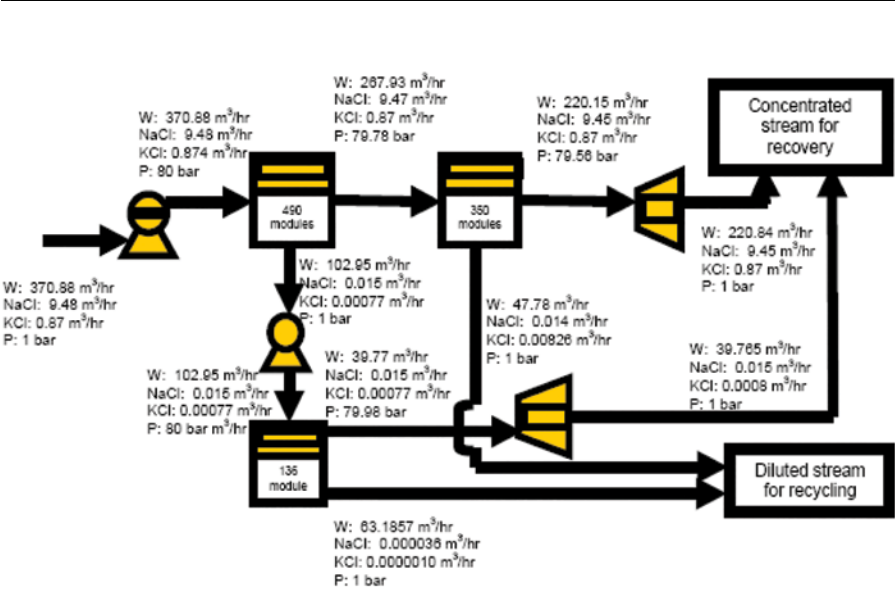


FIGURE 7.6 Optimal RO network for wastewater treatment in pulp and paper processes.

(Adapted from Saif et al., 2013)

7.10 SUPERSTRUCTURE OPTIMISATION OF WATER NETWORK IN A PETROLEUM REFINERY

Khor et al. (2011) investigated the opportunity of reducing water consumption in a petroleum refinery. Buabeng-Baidoo and Majozzi (2015) made further improvements on the work of Khor et al. (2011). A detailed mathematical modelling of a hollow fibre RO network with multiple contaminants is incorporated in a water network model to simultaneously minimise the water consumption and the total annualised cost while optimising the number of RO modules, type, size, connecting pipes, pumps, ERDs, and operating conditions. The water network included water sources, RO stages, and sinks used to treat wastewater. An MINLP optimisation framework

was developed to investigate the optimal water network and evaluate the opportunity of water recycle–reuse and regeneration reuse–recycle. The design of an optimal RO network was achieved using the state-space approach of El-Halwagi (1992).

The MINLP optimisation framework included several data inputs. A set of water and sink sources, a network of RO modules with design specifications, a freshwater source of known pollutant concentration, and a wastewater sink with allowed pollutant concentrations were included in the input data. Also, the RO process constraints, network boxes constraints, and the existence of units (binary variables) were included in the optimisation framework.

The MINLP optimisation framework has resulted in an optimised RO network with notable economic benefits as reported in Table 7.5. Table 7.6 also shows the optimum economic data and model parameters of the water network superstructure.

Four scenarios were considered by Buabeng-Baidoo and Majozzi (2015) to evaluate the feasibility of using regeneration water network superstructure compared to the black box model of linear cost functions of the original water network.

TABLE 7.5
Detailed Operational Data and Economic Data of RO Network

Parameter	Unit	Value
Pure water permeability	(m/s Pa)	5.5×10^{-13}
Shell side pressure drop per module per regenerator	(Pa)	4.05×10^4
Solute permeability coefficient	(m/s)	1.82×10^{-8}
Fibre length	(m)	0.75
Seal length	(m)	0.075
Outside radius of fibre	(m)	42×10^{-6}
Inner radius of fibre	(m)	21×10^{-6}
Membrane area	(m ²)	180
Water viscosity	(kg/m s)	0.001
Dimensionless constant	–	0.69
Permeate pressure per regenerator	(Pa)	101,325
Pump and ERD efficiency	–	0.7
Liquid recovery for all regenerators	–	0.7
Osmotic constant	(Pa)	4.15×10^{-7}
Cost parameter for chemicals	(\$/kg)	0.11
Cost of electricity	(\$/kWh)	0.06
Cost coefficient for pump	(\$/yearW0.65)	6.5
Cost coefficient for turbine	(\$/yearW0.43)	18.4
Cost per module of hollow fibre membrane	(\$/year module)	2300
Max. flow rate per hollow fibre module	(kg/s)	0.27
Min. flow rate per hollow fibre module	(kg/s)	0.21

(Adapted from El-Halwagi, 1997)

TABLE 7.6
Detailed Operational Data and Economic Data of Water Network Superstructure

Parameter	Unit	Value
Annual operating time	h	8760
Unit cost of fresh water	(\$/t)	1
Unit cost of wastewater	(\$/t)	1
Interest rate per year	–	5%
Number of years	(year)	5
Parameter p for carbon steel piping	–	7200
Parameter q for carbon steel piping	–	250
Velocity	(m/s)	1

(Adapted from Buabeng-Baidoo and Majozi, 2015)

- Scenario 1: Base case of only regeneration unit which is included within the water network without RO membranes
- Scenario 2: A single regenerator of RO module is considered within the water network superstructure at constant removal ratio of 95%.
- Scenario 3: Multiple regenerators of RO modules are considered within the water network superstructure at constant removal ratio of 95%.
- Scenario 4: Multiple regenerators of RO modules are considered within the water network superstructure at variable removal ratio.

The results of MINLP optimisation framework for three scenarios are presented in Table 7.7.

Unsurprisingly, Scenario 1 demanded the highest total annualised cost as a result of the highest consumption of fresh water. The associated optimal water network of Scenario 1 is presented in Figure 7.7.

Scenario 2 of single RO membrane (regeneration unit) achieved a decrease in freshwater consumption and wastewater production of around 15.26% and 43.36%, respectively. Also, the total annualised cost of Scenario 2 was lower than Scenario 1 by 17.6%. This is attributed to the use of ERD, which can extract energy from the retentate streams, which in turn reduces the energy usage. The reduction of fresh water and wastewater generation were evaluated based on a simple comparison against the calculated values of the first scenario. The associated optimal regeneration water network based on the distribution boxes of RO network is depicted in Figure 7.8. However, Figure 7.9 presents the optimal regeneration water network at the fixed removal ratio of pollutants of 95%. Scenario 2 of single regenerations of RO modules at fixed 95% of removal ratio has made the optimisation methodology to select 20 hollow fibre RO membranes with one pump and one ERD.

Scenario 3 of multiple regenerations of RO modules at fixed 95% of all pollutants removal ratio has several advantages. This arrangement was already illustrated in Figure 7.10. Scenario 3 achieved a reduction of freshwater consumption and

TABLE 7.7
Comparison between Three Scenarios

Parameter	Unit	Case 1 (no regeneration)	Case 2 (single regeneration at fixed removal ratio)	Case 3 (two regenerators at fixed removal ratio)
Freshwater flow rate	(kg/s)	38.4	32.54	28.87
Wastewater flow rate	(kg/s)	13.4	7.59	3.91
Cost of regeneration	(million \$/year)	–	0.068	0.23
Total annualised cost	(million \$/year)	1.7	1.4	1.32
CPU time	(h)	0	0.13	6

(Adapted from Buabeng-Baidoo and Majozi, 2015)

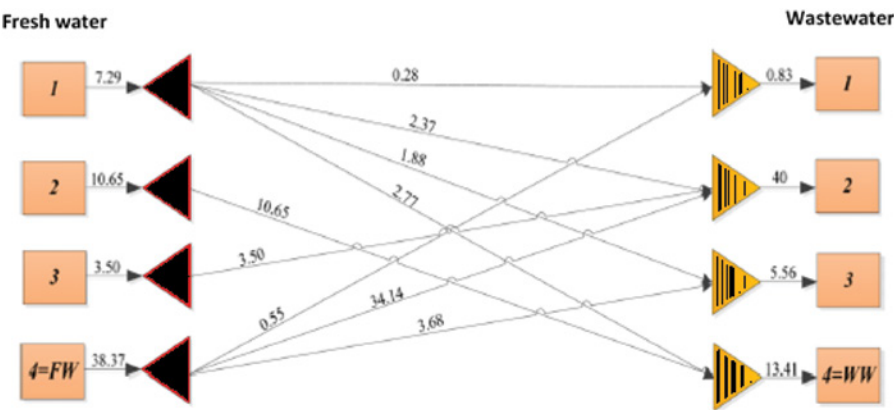


FIGURE 7.7 Optimum water network configuration of Scenario 1.

(Adapted from Buabeng-Baidoo and Majozi, 2015)

wastewater generation of 24.82% and 70.82%, compared to the original case (base case of Scenario 1), and the total annualised cost was reduced by 22.35%. Scenario 3 of multiple regenerators of RO modules and fixed removal ratio of all pollutants of 95% led the MINLP optimisation framework to a solution consisting of two parallel regenerators where each regenerator holds 37 modules, as presented in Figure 7.10.

Scenario 4, which is associated with multiple regenerators of RO modules and a variable removal ratio of pollutants, also has an updated removal ratio of 97% compared to Scenarios 2 and 3. The optimum regenerators water network is schematically shown in Figure 7.11. This case has ended up with two parallel regenerators of 15 hollow fibre RO modules per each regenerator and two pumps and two ERDs. This time, further reductions of freshwater consumption and wastewater generation of 3.12% and 30.43%, respectively, were noted when using Scenario 4 compared to Scenario 3. This corresponded to a 15.91% decrease in the total annualised cost compared to Scenario 3. The freshwater consumption and wastewater generation were

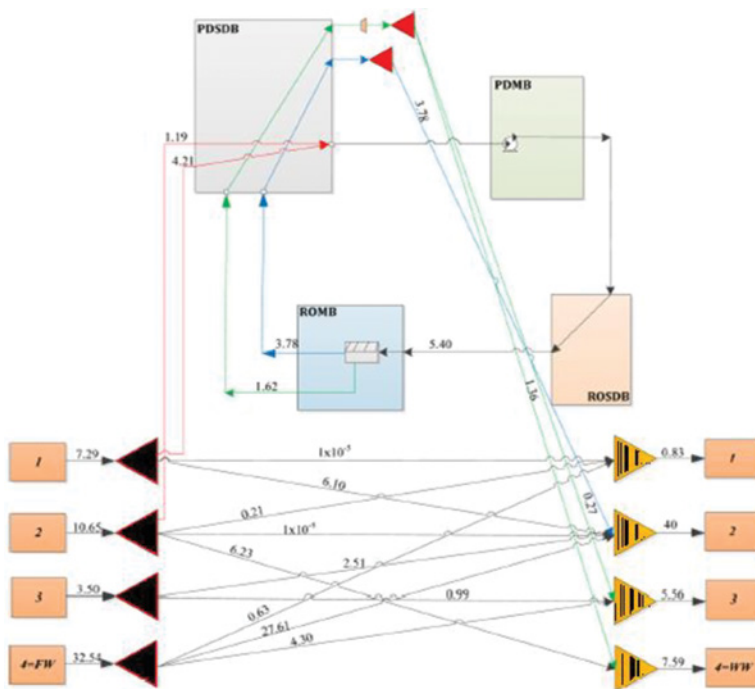


FIGURE 7.8 Optimum regeneration water network of single RO module at constant removal ratio of 95% of Scenario 2 based on the distribution boxes of RO network.

(Adapted from Buabeng-Baidoo and Majozi, 2015)

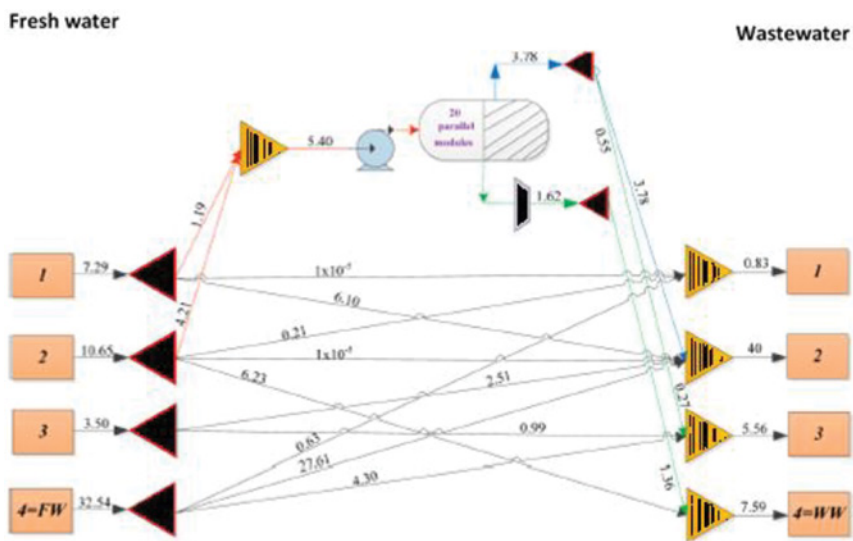


FIGURE 7.9 Optimum regeneration water network of multiple RO module at constant removal ratio of 95% of Scenario 2.

(Adapted from Buabeng-Baidoo and Majozi, 2015)

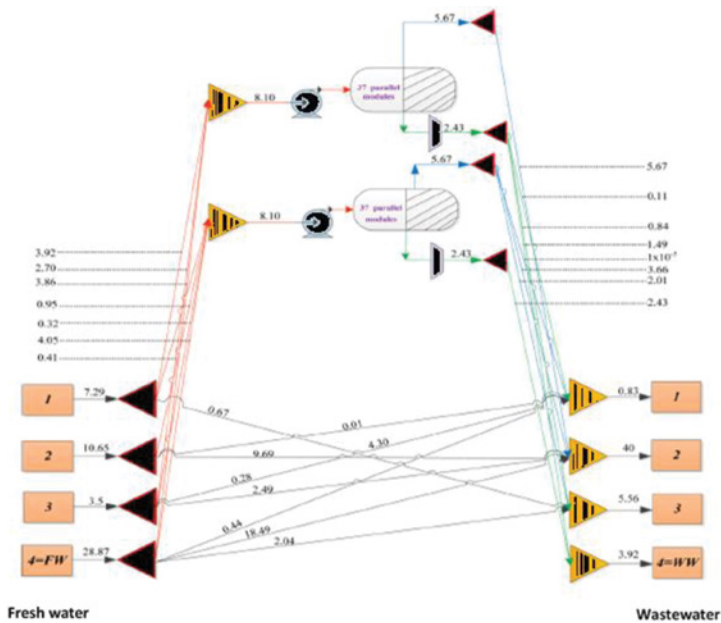


FIGURE 7.10 Optimum regeneration water network of multiple RO module at fixed removal ratio of 95% of Scenario 3.

(Adapted from Buabeng-Baidoo and Majozzi, 2015)

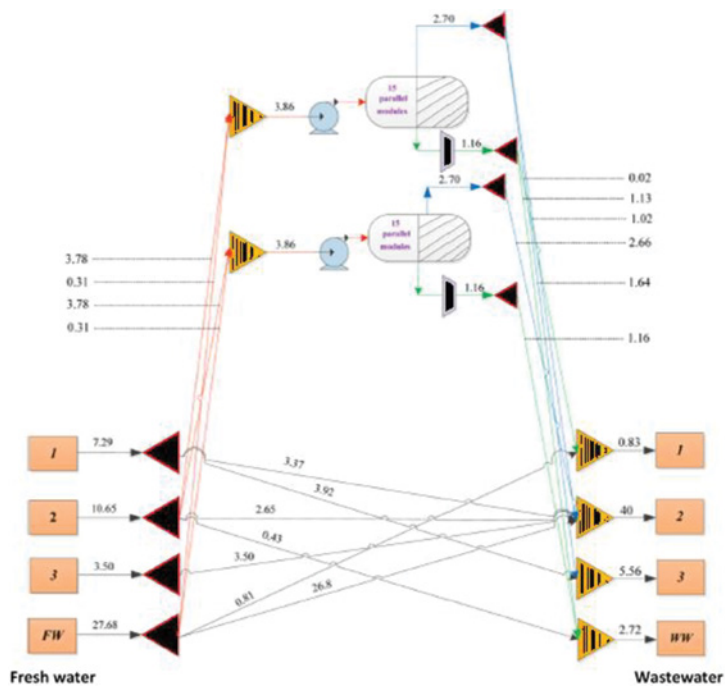


FIGURE 7.11 Optimum regeneration water network of multiple RO module at variable removal ratio of Scenario 4.

(Adapted from Buabeng-Baidoo and Majozzi, 2015)

decreased by 28% and 80%, from Scenarios 3 to 4, albeit with more computational time required to attain the optimal network.

7.11 SUPERSTRUCTURE OPTIMISATION OF THE PULP AND PAPER INDUSTRY USING ELECTRODIALYSIS AND RO MEMBRANES MULTI-REGENERATOR SYSTEMS

Abass and Majozi (2016) studied the synthesis of a superior multi-regenerator membrane network of electrodialysis (ED) and hollow fibre RO processes into an existing pulp and paper industry. The expectation was that the involvement of such an optimised network would reduce the total treatment cost and freshwater consumption in the current high freshwater consumption industry. To attain this goal, Abass and Majozi (2016) developed detailed models for ED and RO regenerator membrane systems. These models were incorporated into the water network model. The multi-regenerator system of ED and RO network was solved using a MINLP optimisation framework which minimises the total annualised cost while optimising a number of design and operating parameters subject to constraints. Abass and Majozi (2016) considered three scenarios of the water network of the pulp and paper industry to highlight the merits of using a multi-regenerator membrane system network in the existing water network.

- Scenario 1: Existing water network of the pulp and paper industry as presented in Figure 7.12 (base case).
- Scenario 2: A model of water network with multi-regeneration membrane systems based on the black box method. A fixed and variable removal ratio was considered here and is shown in Figures 7.13 and 7.14, respectively.
- Scenario 3: Detailed synthesis of multi-regenerator membrane systems and water network considering the targeted objective function. These are presented in Figures 7.15 and 7.16, respectively.

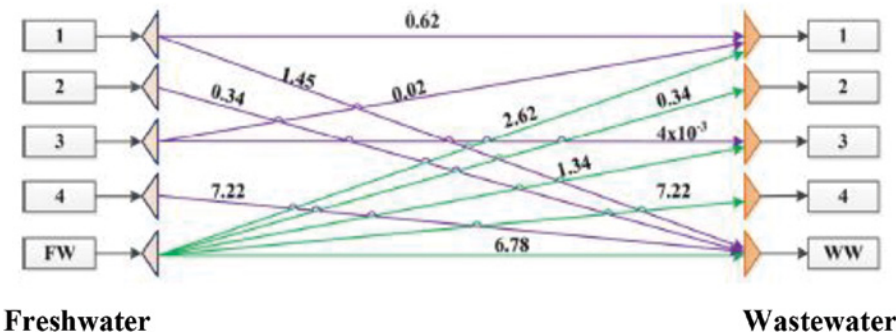
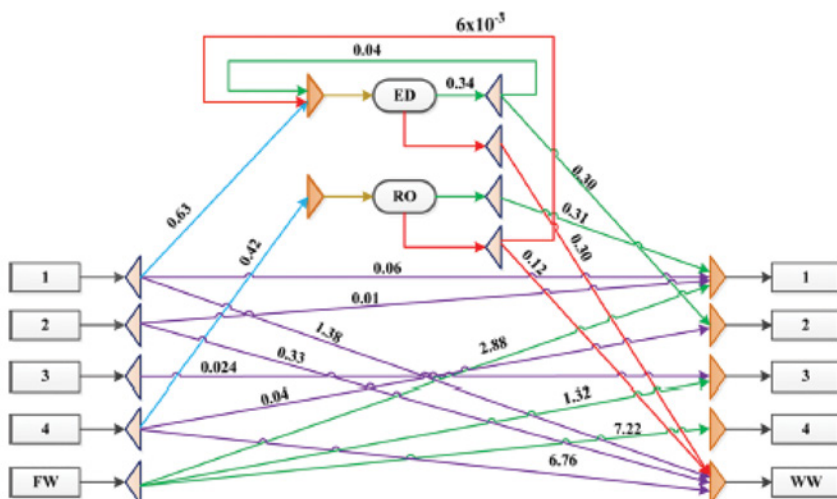


FIGURE 7.12 Optimum water network configuration of pulp and water industry of Scenario 1. (Adapted from Abass and Majozi, 2016)

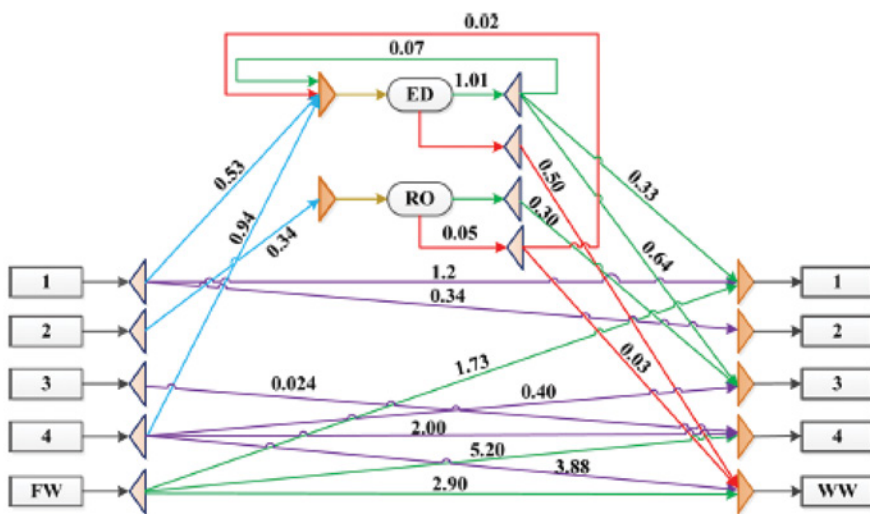


Freshwater

Wastewater

FIGURE 7.13 Optimum water network configuration of multi-regenerator membrane systems and water network of pulp and paper industry at fixed removal ratio of Scenario 2.

(Adapted from Abass and Majozi, 2016).



Freshwater

Wastewater

FIGURE 7.14 Optimum water network configuration of multi-regenerator membrane systems and water network of pulp and paper industry at variable removal ratio of Scenario 2.

(Adapted from Abass and Majozi, 2016).

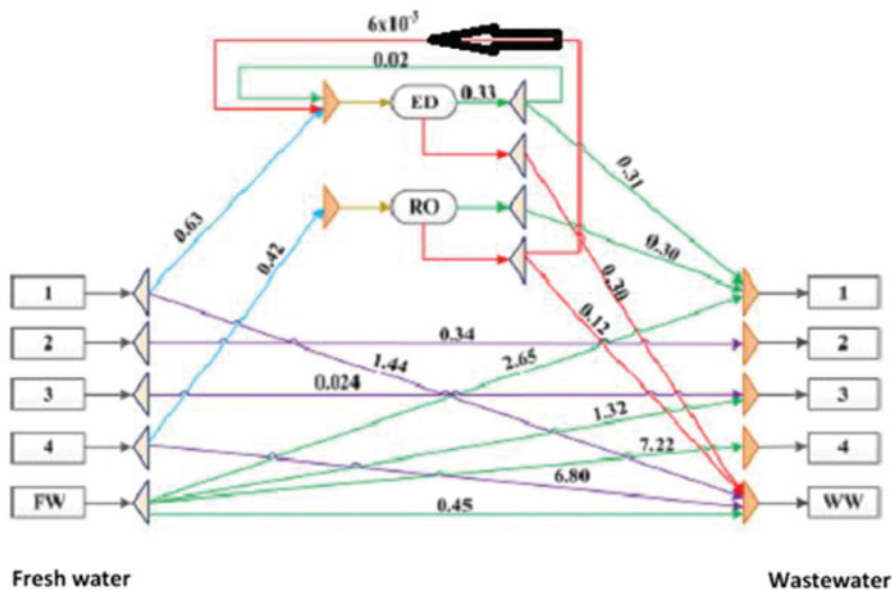


FIGURE 7.15 Optimum water network configuration of multi-regenerator membrane systems and water network of pulp and paper industry at fixed removal ratio of Scenario 3.
(Adapted from Abass and Majoji, 2016)

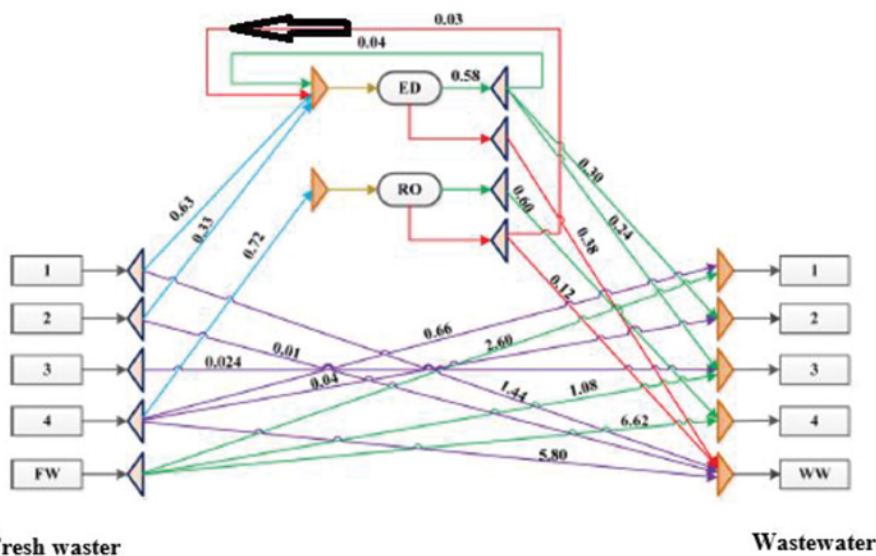


FIGURE 7.16 Optimum water network configuration of multi-regenerator membrane systems and water network of pulp and paper industry at variable removal ratio of Scenario 3.
(Adapted from Abass and Majoji, 2016)

A comparison between the performance of these proposed scenarios readily reveals that the black box approach provided inaccurate costing compared to that obtained by using the detailed models. Moreover, the black box model failed to provide an accurate insight on the total usage of energy for the optimal network. Finally, the embedding of multi-generator ED and RO membrane systems into the water network of pulp and paper industry reduced the cost by 46%, freshwater consumption by 43.7%, and wastewater generation by 50.9%.

7.12 THE USE OF A REGENERATED WATER NETWORK FOR OPTIMUM WATER CONSUMPTION IN THE DAIRY INDUSTRY

Buabeng-Baidoo et al. (2017) evaluated the feasibility of employing an RO process to treat the wastewater from the raw milk processing department (RMPD) of Amul Dairy (India) with a prime objective of reducing the freshwater consumption of the plant. The RMPD consumes a substantial amount of water. An MINLP-based optimisation framework was therefore developed to predict the best water network which would reduce water consumption and improve wastewater generation. The regeneration unit of the RO membrane was added to the water flowsheet connecting the water sources box (producing water) and water sinks box (consuming water) as depicted in Figure 7.17. The network was very similar to that considered by Khor et al. (2011).

A detailed mathematical model was developed for each unit, where the complete RO process and cost functions were taken from El-Halwagi (1997), as previously reported in Table 7.5. Several scenarios involving a hollow fibre RO network in the

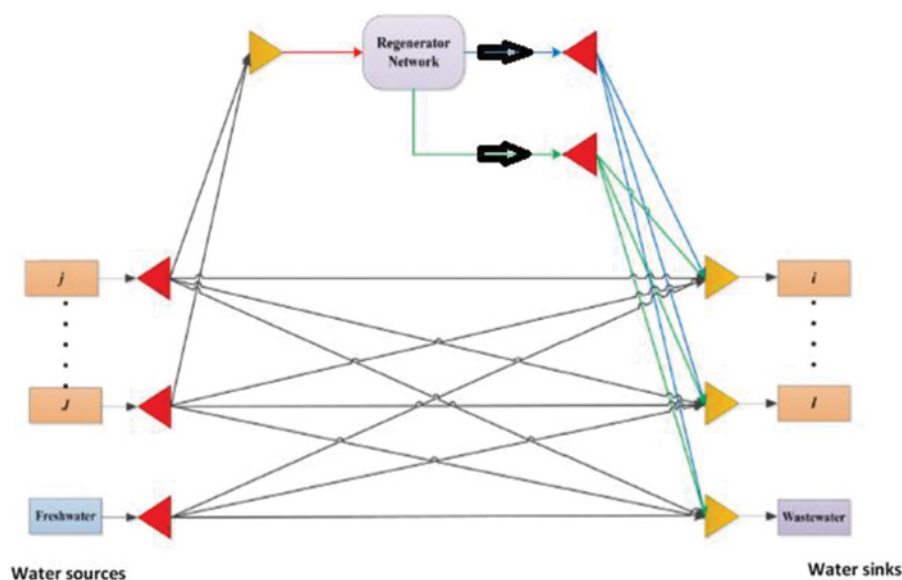


FIGURE 7.17 General representation of regeneration water network.

(Adapted from Buabeng-Baidoo et al., 2017)

existing water network of dairy plant were considered by Buabeng-Baidoo et al. (2017). The following scenarios were considered for the study:

- Scenario 1: a water network without an RO membrane unit, no water is reused or recycled, and there is no interconnection between the units (base case, Figure 7.18).
- Scenario 2: a water network without an RO membrane unit but with wastewater recycling resulting in complicated interconnections between the different units (Figure 7.19).
- Scenario 3: a water network with an RO membrane as a regeneration unit for water reuse and recycling (Figure 7.20). In other words, wastewater from the milk department was decontaminated by an RO membrane and recycled to the same department for cleaning the process equipment.

The optimisation results of this study are given in Table 7.8, which shows a performance comparison between the three proposed scenarios. Scenario 1 has the highest freshwater consumption, wastewater generation, and treatment cost. The optimal water network of the base case is presented in Figure 7.18.

Figure 7.19 shows the optimal water network of Scenario 2, which encompasses unit connections in an integrated process but without the regeneration unit and water reuse. This scenario resulted in lower freshwater consumption and wastewater generation compared to the base case (Scenario 1) with a reduction of 21%, 54%, and 27% in freshwater consumption, wastewater generation, and total annualised cost,

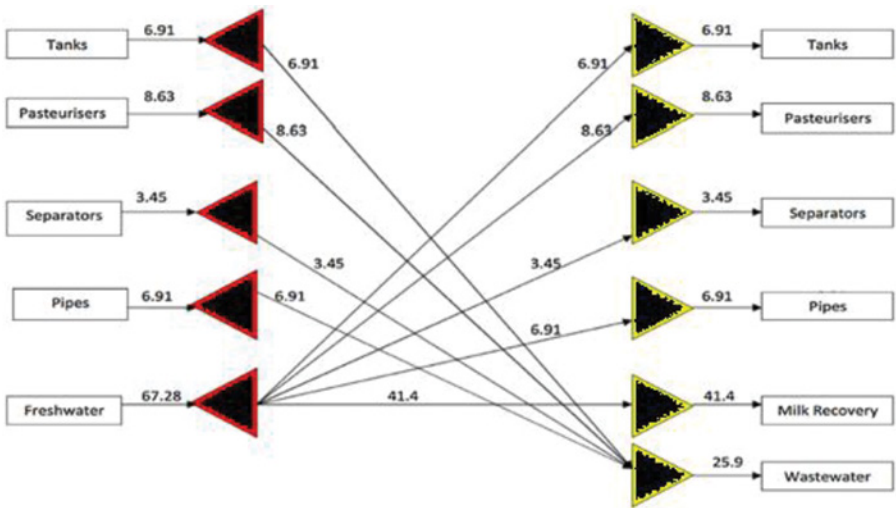


FIGURE 7.18 Optimal water network of Scenario 1.

(Adapted from Buabeng-Baidoo et al., 2017)

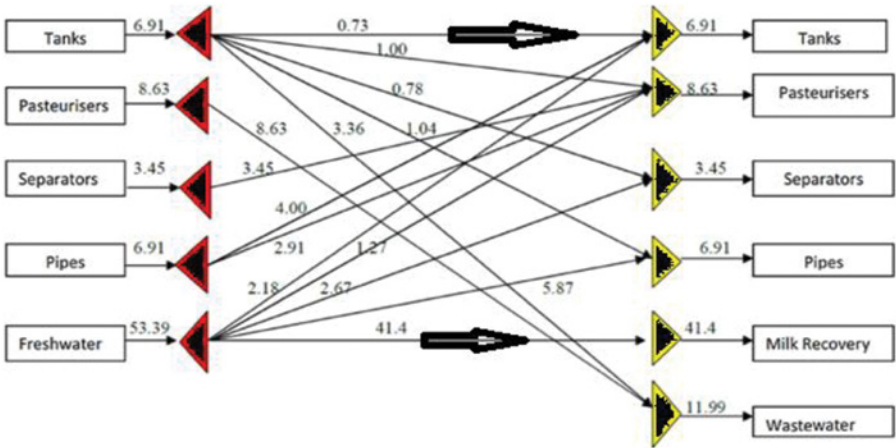


FIGURE 7.19 Optimal water network of integrated units without regeneration unit of Scenario 2.

(Adapted from Buabeng-Baidoo et al., 2017)

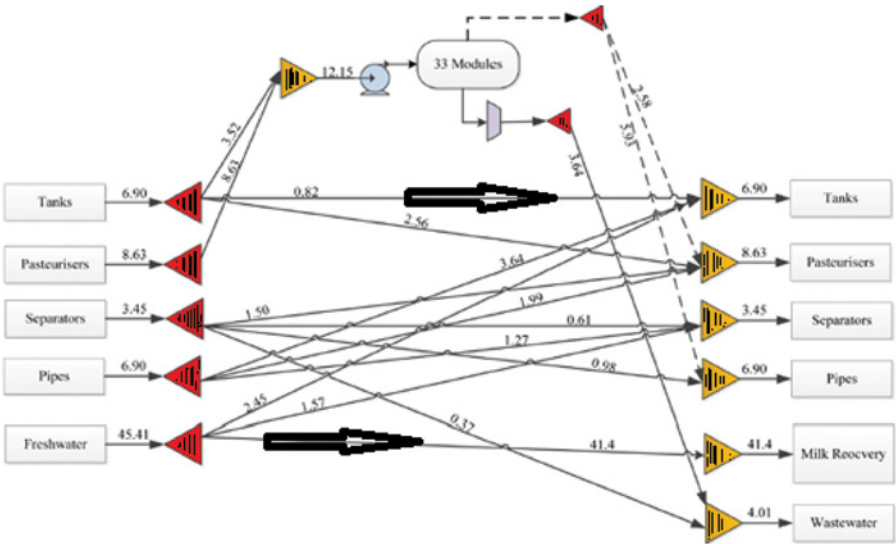


FIGURE 7.20 Optimal water network of integrated units with regeneration unit of Scenario 3.

(Adapted from Buabeng-Baidoo et al., 2017)

respectively. The optimal regeneration water network of Scenario 3 (Figure 7.20) used 33 RO parallel modules, one pump, and one ERD. It resulted in the reduction of 33% of freshwater consumption, 85% of wastewater generation, and 33% of treatment cost compared to the base case (Scenario 1).

TABLE 7.8
MINLP Optimisation Results of Three Scenarios

Parameter	Unit	Scenario 1 (base case)	Scenario 2	Change from Scenario 1	Scenario 3	Change from Scenario 1
Fresh water	(kg/s)	67.28	53.39	(−21%)	45.41	−33%
Wastewater	(kg/s)	25.9	11.99	−54%	4.01	−85%
Total annualised cost	(million \$/ year)	2.94	2.15	−27%	1.96	−33%

(Adapted from Buabeng-Baidoo et al., 2017)

7.13 OPTIMAL RO NETWORK CONFIGURATION FOR THE REMOVAL OF DIMETHYLPHENOL FROM WASTEWATER

Al Obaidi et al. (2018) used simulation studies to assess the performance of different configurations of multistage RO process, consisting of three modules of spiral wound RO membranes (HM4040-LPE, Ion Exchange, Mumbai, India), for the removal of dimethylphenol from wastewater at different feed concentrations (Chapter 6). The schematic diagram of the proposed designs of multistage RO process and the simulation results are given in Figure 7.21. Instead of using a superstructure optimisation, Al-Obaidi et al. (2018) considered a single objective, based on a non-linear programming optimisation problem, to obtain the optimal module configuration and operating conditions which would yield the highest dimethylphenol rejection for each of the configurations shown in Figure 7.21. The process model for this study has already been discussed in Chapters 5 and 6. However, an additional set of mathematical equations, which describe the whole mass and solute balance and the interaction between RO stages, pressure vessels, and main streams, have been used. These are given as follows:

$$Q_{f(plant)} = Q_{r(plant)} + Q_{p(plant)} \quad (7.1)$$

$$Q_{f(plant)} C_{f(plant)} = Q_{r(plant)} C_{r(plant)} + Q_{p(plant)} C_{p(plant)} \quad (7.2)$$

$$Q_{r(plant)} = Q_{r(s=n)} \quad s: \text{refers to stage and } n \text{ signifies number of the used stages} \quad (7.2)$$

$$Q_{p(Plant)} = \sum_{s=1}^n Q_{p(s)} \quad (7.3)$$

$$C_{r(plant)} = C_{r(s=n)} \quad (7.4)$$

$$Rej_{(plant)} = \frac{C_{f(plant)} - C_{p(plant)}}{C_{f(plant)}} \times 100 \quad (7.6)$$

$$Rec_{(plant)} = \frac{Q_{p(plant)}}{Q_{f(plant)}} \times 100$$

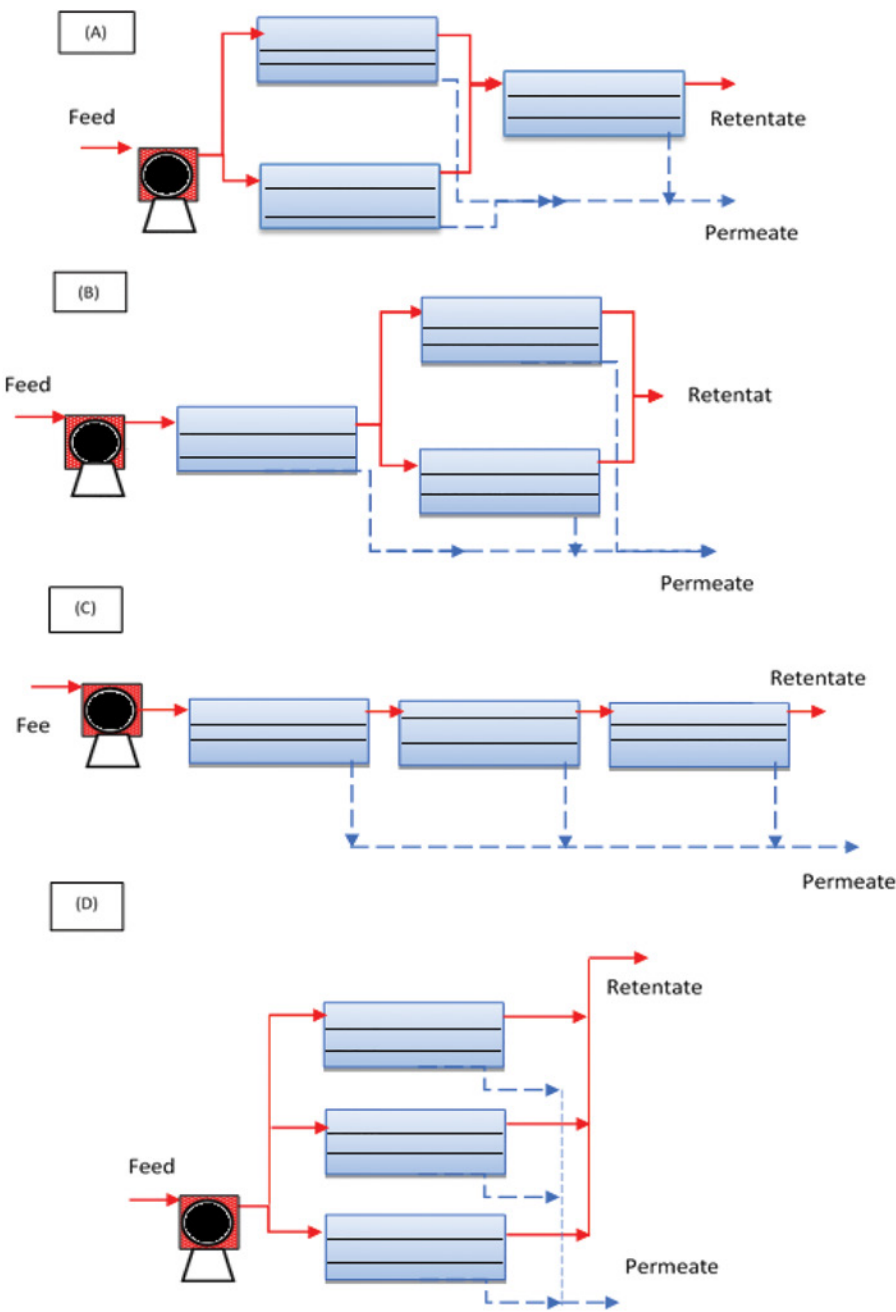


FIGURE 7.21 Schematics of different RO configurations.

(Adapted from Al-Obaidi et al., 2018a)

7.13.1 OPTIMISATION PROBLEM DESCRIPTION AND FORMULATION

For each of the configurations in Figure 7.21, the optimization problem is described mathematically as:

Max Rej (dimethylphenol)

$Q_{f(plant)}, P_{f(in)(plant)}, T_{(plant)}$

Subject to:
Equality constraints:
Process model: $f(x, u, v) = 0$
Inequality constraints:

$Q_{f(plant)}^L \leq Q_{f(plant)} \leq Q_{f(plant)}^U$

$P_{f(in)(plant)}^L \leq P_{f(in)(plant)} \leq P_{f(in)(plant)}^U$

$T_{b(plant)}^L \leq T_{b(plant)} \leq T_{b(plant)}^U$

The optimisation problem involves the following upper and lower bounds of an individual spiral wound RO membrane based on the manufacturers’ specifications:

$Q_f^L \leq Q_f \leq Q_f^U$

$P_{b(in)}^L \leq P_{b(in)} \leq P_{b(in)}^U$

$T_b^L \leq T_b \leq T_b^U$

The optimisation problem maximises the dimethylphenol rejection while optimising the operating conditions, such as inlet feed flow rate ($Q_{f(plant)}$), pressure ($P_{f(in)(plant)}$), and temperature ($T_{(plant)}$) for a given set of inlet feed concentrations. The three different inlet feed concentrations considered were 1.637, 2.455, and 6.548 kmol/m³.

The optimisation is subjected to a number of upper and lower bounds of decision variables, which include the operating pressure, the flow rate, and the temperature. This optimisation takes into account the pressure drop in each element of 1.38 atm along the membrane length as a critical constraint based on the recommendations of

TABLE 7.9
Permissible Values of Operating Conditions of Membranes Type HM4040-LPE, Ion Exchange, Mumbai, India

Parameter	Permissible value	Parameter	Permissible value
Max. feed temperature (°C)	40	Max. feed pressure (atm)	24.77
Max. pressure drop per element (atm)	1.3817	Max. and min. feed flow rate (m³/s)	1E-4 – 1E-3

the membrane manufacturer. Also, the optimisation considered the lower and upper limits of the membrane constraints of inlet pressure, flow rate, and temperature as given in Table 7.9.

7.13.2 OPTIMISATION RESULTS AND DISCUSSION

The optimisation results with maximum dimethylphenol rejection for the four selected RO networks and the three different feed concentrations are given in Table 7.10. This also shows the maximum pressure loss occurring in the RO element and the total pressure loss for the whole layout. Table 7.10 also includes the optimum values of the operating conditions for each layout.

The optimisation results shown in Table 7.10 clearly show that the four tested RO configurations accomplished a dimethylphenol rejection between 95.6% and 99.25% at different optimal operating conditions. This shows that the specific optimum operating conditions are important for each RO layout for achieving the maximum dimethylphenol rejection while being constrained within the allowed pressure drop per each element of 1.38 atm. Additionally, the operating temperature maximum limit was important for all RO configurations to attain the objective function. Table 7.10 shows that the parallel layout D achieves the highest dimethylphenol rejection for all feed concentrations. Interestingly, the optimisation results confirmed the necessity of lowering the inlet feed flow rate in order to keep the filtration process within the allowable pressure drop, which in turn maximised the removal efficiency.

TABLE 7.10
Optimisation Results of Dimethylphenol for Four Scenarios of RO Networks

Operating concentration (x10 ³ kmol/m ³)	Layout	Optimum decision variables (operating conditions) $Q_{f(plant)}$ (m ³ /s)		Max. pressure loss of element (atm)	Total pressure loss of the layout (atm)	Rej_{plant} (maximum rejection) %
		$P_{f(in)(plant)}$ (atm)				
1.637	A	4.511E-4	20.27	1.38	2.456	98.35
	B	2.065E-4	15	1.38	1.639	96.92
	C	2.065E-4	15	1.38	2.140	95.59
	D	7.224E-4	24.77	1.38	1.376	98.97
2.455	A	4.595E-4	21.75	1.38	2.375	98.54
	B	2.057E-4	15	1.38	1.647	97.26
	C	2.057E-4	15	1.38	2.183	96.20
	D	7.179E-4	24.77	1.38	1.375	99.05
6.548	A	4.519E-4	21.96	1.38	2.491	98.90
	B	2.025E-4	15	1.38	1.676	97.88
	C	2.025E-4	15	1.38	2.342	97.34
	D	7.013E-4	24.77	1.37	1.372	99.25

$T_{(plant)} = 40^{\circ}\text{C}$
(Adapted from Al-Obaidi et al., 2018)

Broadly speaking, lowering the inlet feed flow rate has a substantial positive impact on reducing the pressure drop along the membrane length due to lowering the friction intensity. According to Table 7.10, the high operating pressure was in fact an important parameter for layouts A and D for maximising the rejection compared to layouts B and C. The rationale behind this is that the use of a higher feed flow rate in layouts A and D requires a higher feed pressure to compensate for the loss of pressure in such layouts. It is worthy to note that layouts B and C operated at the lowest possible operating pressure and produced marginally lower dimethylphenol rejections.

To sum up, the optimisation results revealed that a parallel layout can yield the maximum dimethylphenol rejection within the lowest pressure loss compared to other layouts investigated.

7.14 CONCLUSIONS

Reverse osmosis (RO) has been successfully applied in many wastewater treatment industries as a highly efficient separation process. Model-based optimisation techniques can be very valuable for determining optimal process network and operating variables, which can be used to achieve several objectives such as minimum cost, maximum rejection, and minimum energy.

This chapter has reviewed several studies which have focused on the synthesis of an RO network integrated within an overall water network in a number of industrial applications.

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8 Optimisation of an RO-Based Wastewater Treatment Process Using Genetic Algorithms

8.1 INTRODUCTION

Genetic algorithms (GA) is a stochastic search method which imitates the natural biological evolution process. The GA methodology provides one of the best tools for finding optimal solutions for several industrial problems such as seawater desalination and wastewater treatment, and this is due to its consistency, speed, and flexibility for quickly reaching a global solution. This chapter discusses examples of successful applications of the GA methodology on seawater desalination studies. In particular, it also discusses the application of GA for maximising the removal of organic compounds from wastewater in an RO process.

8.2 GENERAL CONCEPTS OF GENETIC ALGORITHM AND EVOLUTIONARY ALGORITHMS

The genetic algorithm methodology is an adaptive search method used to locate the exact or approximate optimum solution for a specified process based on natural evolution. Holland (1975) originally developed the basics of GA as a stochastic and population-based optimisation approach, which was constructed on the perceptions of natural evolution and the biological metaphor of natural selection. Holland (1975) confirmed that the use of GA, as an optimisation method, could yield better results in several applications compared to other conventional optimisation methods. More specifically, the implementation of simple genetic algorithm (SGA) is extensively used as an optimisation tool in several applications to gain global and local optimal solutions for different processes (Leardi, 2001; Soleimani et al., 2013). For example, Figure 8.1 presents several local and global optimal maximum and minimum solutions for a given two-dimensional function f (Weise, 2009).

8.2.1 GENERALISED GENETIC ALGORITHM

GA can be used to handle most mathematical models and can produce a highly efficient correlation tree based on GA parameters, such as mutation and crossover, which

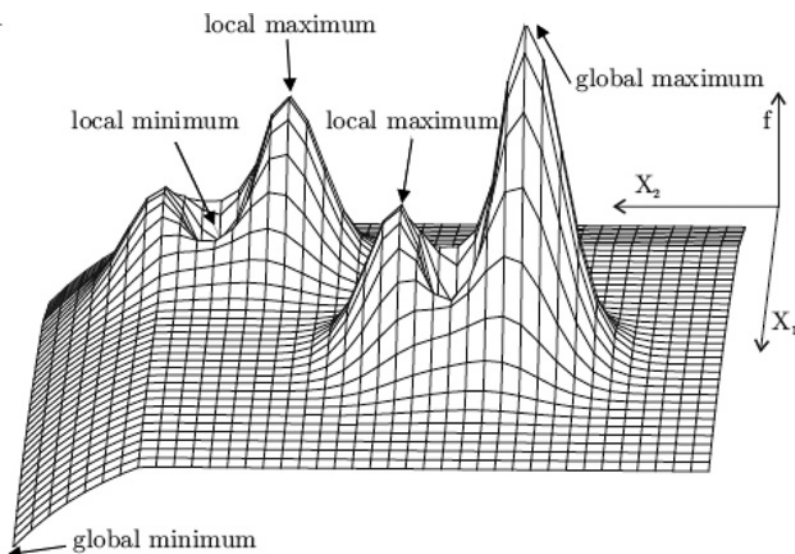


FIGURE 8.1 Minimum and maximum global and local optimal solutions of a given function.

(Adapted from Weise, 2009)

can closely predict the mathematical behaviour of a function (Kumar et al., 2010). GA has been successfully applied in a wide range of chemical engineering applications, including design and operation such as distillation (Fraga and Senos Matias, 1996), semi-batch reactor (Raj Gupta and Gupta, 1999), steam reforming of hydrocarbons for the generation of hydrogen and synthesised gas (Rajesh et al., 2000), hydrogenation reaction system (Victorino et al., 2007), and microchannel reactor to synthesise liquid hydrocarbons (Na et al., 2017).

The GA methodology uses the population of several points simultaneously (population of solution candidates) along with probabilistic operators, reproduction, crossover, and mutation, as inspired by natural genetics. The initial GA solution is randomly selected from the population in an optimised space, and the convergence to a proper solution is carried by applying three operators of reproduction, crossover, and mutation in an iterative manner.

By using such operators, individuals are selected at random from the current population at each step and become parents. These are then used to produce the next generation of children and so on, and the population “evolves” toward an optimal solution.

8.2.2 SIMPLE GENETIC ALGORITHM

The solution of SGA is carried out by considering a weighted average of several contradictory objective functions, which need to be optimised simultaneously in the presence of a few constraints. The SGA technique has several advantages, including the fact that it does not need initial values for the decision variables.

These need to be coded as a series of binary numbers during the optimisation process. They are then recoded into real numbers and used in the model equations. This may increase the computing time required to speed up the convergence rate (Deb et al., 2002).

Most engineering optimisation problems can readily be very complex as they are multimodal and can have a variety of constraints. Usually, fast GA software tools are used to find the best possible solution for a given problem (Weise, 2009).

Goicoechea et al. (1982) found that, in some cases, when optimising a single-objective function, certain optimal solutions can be lost, especially when there is a considerable gap between the objective functions. This is why a singular optimum process solution may not reflect the true optimum solution.

8.2.3 NON-DOMINATED SORTING GENETIC ALGORITHM (NSGA)

Several researchers attempted to enhance the performance of the GA algorithm in order to cope with multimodal problems and not be constrained to a local solution. In this respect, several approaches have been used to solve multimodal problems, including crowding (De Jong, 1975), fitness share (Goldberg et al., 1987), clearing (Pétrowski, 1996) and multi-national GA (Ursem, 1999). Others, such as Deb et al. (2002), investigated the non-dominated sorting genetic algorithm (NSGA). This type of GA has introduced for the first time the concept of elitism. Elitism essentially means the selection of the favoured members generated from the crossover and mutation of the parents, which can be used later for the next generation. Therefore, an elitist would guarantee at least one copy of the best individuals (one global solution) of the existing generation onto the next generation. However, with this method, there is a high possibility of generating local optimum solutions, which is one of the pitfalls of this methodology (Weise, 2009). The performance of NSGA is comparable to that of the simple solution of basic genetic algorithm (SGA) (note, SGA focusses on optimisation problems with a single-objective function). Basic multi-objective optimisation formulations (mostly contain conflicting aims) can be solved using the NSGA. This can be used to explore several optimum and non-dominated solutions of the proposed process. A multi-objective optimisation problem can include several objective functions, which can be used to minimise or maximise the targeted variables. This frees the decision-maker from being narrowed down to a single optimal solution, and the final judgement can be made after examining a set of effective and refined solutions.

8.2.4 SPECIES CONSERVING GENETIC ALGORITHM (SCGA)

Li et al. (2002) and Li and Wood (2009) investigated the species conserving GA (SCGA) approach. This also can generate multiple solutions for the specified optimisation problem at the end of each iteration compared to SGA, which generates a single solution. Another distinct advantage of SCGA is the possibility of selecting the most favoured solution for each operation data input without the need of having initial guesstimate values for the decision variables (Guria et al., 2005).

The procedure for solving an optimisation problem is achieved using the following steps:

- The initialisation and selection of the population size: this is a randomly generated initial population of coded strings as a number of individuals within the upper and lower bounds of the decision variables. The number of initial populations is based on the problem type and is usually in the hundreds. An individual can be presented as a vector of real numbers of decision variables. The principle of selection is to randomly take individuals from the existing generations (populations) and copy them to breed a new generation based on their fitness values using a fitness function. Specifically, an individual with a higher fitness will have a greater probability to survive in the next generation. There are several popular classes and functions of population size selection, such as the tournament selection method and the roulette-wheel selection method. The selection approach is therefore dependent on the algorithm chosen and its independent application. A roulette-wheel selection method (Figure 8.2) can be used to select individuals from the current population. Assuming F_i is the fitness of considered individuals i , and N_p is the population size, thus, its probability (P_i) of being selected can be estimated as:

$$P_i = \frac{F_i}{\sum_{j=1}^{N_p} F_j} \quad (8.1)$$

A proportion of a wheel is allocated to each individual i , depending on their fitness or selection probability. Specifically, the roulette-wheel method is characterised by the selection of a random number between 0 and 360, corresponding to how many angles the wheel will rotate. An individual, as pointed by the arrow in Figure 8.2, will be selected and copied to the next

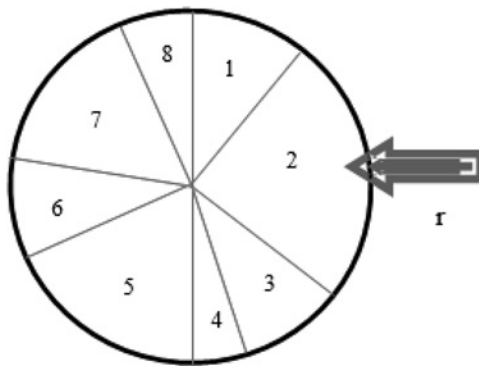


FIGURE 8.2 Roulette-wheel selection.

(Adapted from Al-Obaidi et al., 2017)

generation until Np individuals have been selected. This means that an individual with a higher fitness takes up more area and has therefore a higher probability to be selected (Figure 8.2).

- **Fitness:** this is achieved by computing the fitness of a coded string to the objective function (to be maximised or minimised) by the crossover operator. This is used to select parents from the new formulated population in order to generate offspring with a specified probability P_c . The crossover method is based on the representation of individuals. Therefore, the GA algorithm contains a single-point crossover (0.6 to 1) and a uniform crossover (0.5). For instance, if individuals are represented as chromosomes, the crossover method could be a one-point or a two-point crossover. However, for the case of representing individuals as a vector of real numbers, the crossovers are achieved as an intermediate recombination. Therefore, the offspring O of a randomly chosen parent S and T can be stated as follows:

$$x_0 = x_T + U(x_S - x_T) \quad (8.2)$$

Where, U is a uniformly distributed random number between 0 and 1. Interestingly, the fitness would include the individual's density and niching information as well as providing its rank in the existing population (Weise, 2009). Minimising fitness values would progressively aid in locating a solution candidate. In this respect, the fitness assignment approach can significantly enhance the GA performance to find an optimum solution. It is important to mention that the fitness assignment approach is usually completed before the selection. The final decision of selection is entirely based on the fitness of the specified individuals.

- **Mutation:** this is used to allow a randomly chosen individual to move to a new position with a specified probability (P_m), and mutation is therefore achieved on a single chromosome. This is referred to as the elitism method, which is used to copy the best chromosome to the new population and which holds many of the characteristics of its parents (biology inspired). This relies on random variations of the assigned individuals' genotype and ultimately increases the performance of GA due to its keeping the best solutions. The parent selection of mutation is quite similar to the method of selecting parents for crossover. The corresponding variable will be mutated by using the uniform mutation as shown in Eq. (8.3) after selecting a parent, and a random number, j , of the dimension of decision variables between 1 and m .

$$X'_j = x_j + R(x''_j - x'_j) \quad (8.3)$$

Where, R is a uniformly distributed random number between (-1 and 1), which represents the lower and upper bounds of variable j . More importantly, the next generation population of individuals produced by the mutation parameter, such as sexual reproduction, has a higher degree of fitness and holds two parental genotypes compared to the previously generated population of one genotype.

The aforementioned three GA steps are repeated to generate successive solutions. This evolutionary process continues until fulfilling a specified stopping condition (termination) such as the use of a maximum number of generations or acceptable or highest marked fitness. Eventually, the best individual is assigned and marked as the output of GA operation. It can therefore be said that the GA is based on traditional independent computations, which are controlled by a probabilistic strategy. One of the main advantages of GA methodology is that it can be used as an effective tool for solving an optimisation problem with non-differentiable and discontinuous objective functions that cannot be easily found by gradient-based methods such as Gauss-Newton (Allen and Karjalainen, 1999).

The steps of solving the GA problem are given in Figure 8.3, while Figure 8.4 shows a brief flow chart of the GA steps as discussed previously. The GA approach is considered as a global and popular evolutionary computation optimisation technique (Kumar et al., 2010), while gradient-based methods can only find a local solution.

The GA methodology has been used as a superior optimisation method for maximising the rejection of several highly toxic chemicals from wastewater using an RO system. This is described in more detail in the next sections of this chapter.

The steps for solving an optimisation problem using the species conserving genetic algorithm can be found in the pseudo code by Li et al. (2002) and is presented in Figure 8.5. The SCGA steps are described in the next sections.

Firstly, several species are acknowledged from a specific population size. In SCGA, a species si is the significant term that is assigned as a set of similar individuals with similar characteristics and dominated by its species seed x^* (the best individual). Specifically, the dominated species has the best fitness value (objective value), if for everyone $y \in si$.

$$d\left(x^*, y\right) < r_s$$

(8.4)

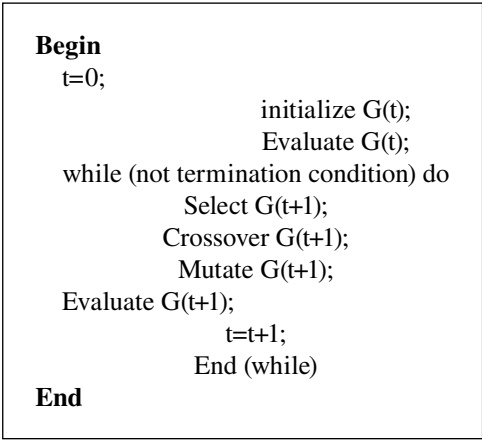


FIGURE 8.3 GA procedure.
(Adapted from Al-Obaidi et al., 2017)



FIGURE 8.4 Flow chart of GA steps.

$$f(y) \leq f(x^*) \tag{8.5}$$

$d(*,*)$ denotes the distance between two individuals and r_s is the species radius. The 2D possible distribution of species is shown in Figure 8.6. A species consists of some individuals and is a part of the feasibility region. Also, some individuals may be found in the intersection of several species.

A population is dynamically divided into a set of subgroups, called species. Each species seed is a possible solution. The objective of the SCGA is to locate a given species which will survive to the next generation. The SCGA has three additional operators in addition to those of a simple GA.

Begin

$t = 0$

Initialize $G(t)$;

Evaluate $G(t)$;

while (not termination condition) do

 Determine species seeds X ;

 Select $G(t+1)$;

 Crossover $G(t+1)$;

 Mutate $G(t+1)$;

 Evaluate $G(t+1)$;

 Conserve species form X , in $G(t+1)$;

$t = t+1$;

end (while)

Identify global optima;

End

FIGURE 8.5 The pseudo codes of the SCGA.

(Adapted from Al-Obaidi et al., 2018)

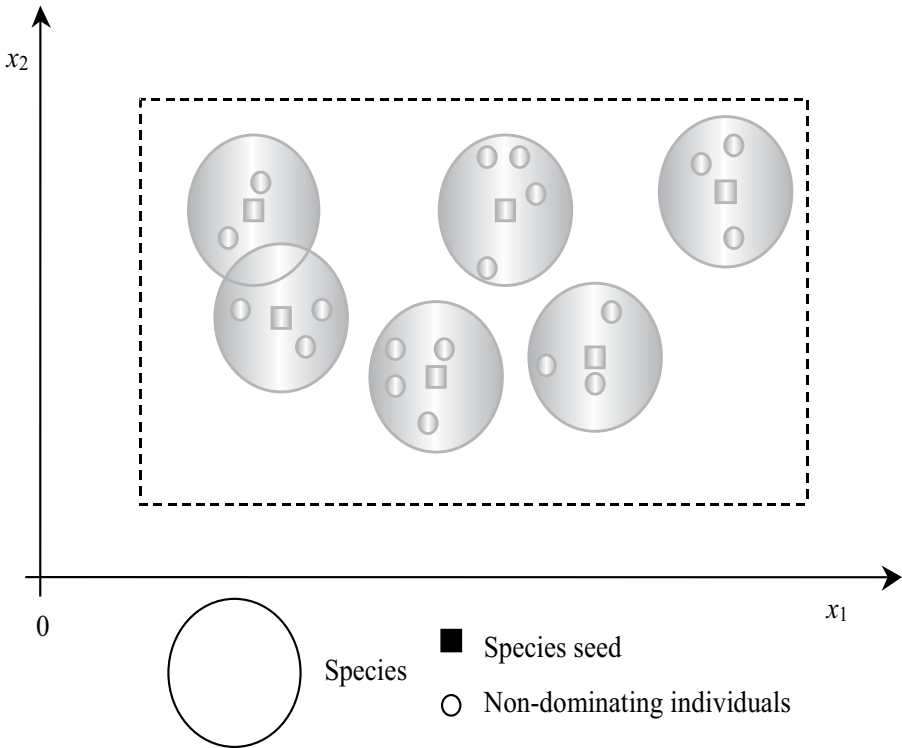


FIGURE 8.6 Species distribution in a 2D space.

(Adapted from Al-Obaidi et al., 2018)

- Finding species seeds: this is used to identify all the possible species from the current population size. Firstly, all the individuals are set as unprocessed. This is followed by selecting the best unprocessed individual to generate a species seed of one species. An individual will be assigned as the associate of the species if its distance to the species seed is less than the species radius and marked as “processed.” This process will be continued until all the individuals have been marked.
- Conserving species seeds: the selected species seed will be copied back to the population and replace the nearest individual if it represents a favourable individual. This in turn will guarantee the species that can survive in the next generation.
- Finding global solutions: the best individual in a species is saved in the set xs . The selection of the best species from xs would be the simple way to recognise the solutions. A threshold r_f ($0 < r_f \leq 1$) is implemented to locate the global solutions. A species seed x is treated as a solution, in case of:

$$f(x) \leq f_{max} - (f_{max} - f_{min})r_f \quad (8.6)$$
 f_{min} and f_{max} are the best and worst objective values, respectively. The default value of species radius is set as considered to be 1.

More details and general information of evolutionary genetic algorithm and several areas of application can be found in Weise (2009).

8.3 APPLICATION OF GENETIC ALGORITHMS FOR OPTIMISING AN RO DESALINATION PROCESS

Several attempts can be found in the literature about the application of GA for the optimisation of an RO-based desalination process. Some of these attempts are discussed in this section.

Guria et al. (2005) used GA for their multi-objective optimisation study to maximise the water flux and minimise both the permeate concentration and filtration cost of a spiral wound and tubular brackish and seawater desalination RO process. The results showed several equally good Pareto results, where the minimisation of the permeate concentration was achieved at a lower solute permeability. However, the maximisations of water and solute permeabilities were supposed to maximise the water flux.

Murthy and Vengal (2006) used GA with the irreversible thermodynamic transport model of Spiegler and Kedem to maximise the rejection of NaCl. They used a laboratory-scale RO desalination system and considered a variable feed flow rate and water flux with a fixed feed concentration. The optimal solution was found at the eighth generation. Moreover, the impact of variable GA parameters such as population, mutation, and crossover probability were studied on the process performance, as they significantly affected the outcome.

GA was also used by Djebedjian et al. (2008) to optimise the performance of a real RO seawater desalination plant in Egypt. The single optimisation objective used was to maximise the water flux by maintaining the best pressure difference across the membrane subject to given constraints on the permeate concentration.

Lee et al. (2009) used GA to predict the membrane fouling of a pilot-scale micro-filtration (MF) membrane drinking water production system using data from the feed flow rate, feed quality, and filtration time. Hwang et al. (2009) also developed a GA model for the prediction of the membrane fouling index in a pilot-scale drinking water hollow fibre membrane filtration system based on the feed flow rate, filtration time, turbidity, temperature, and algae pH over a period of 12 months.

Kim et al. (2009) used GA to develop two functional models for the water flux and salt passage based on the experimental data of the Fujairah seawater desalination RO plant. The models were used to predict the optimum temperature required to maximise the total water recovery rate at the steady state conditions of permeate concentration of 600 ppm TDS.

Renewable energy sources (RES) such as solar and wind have been widely implemented to provide energy for RO membrane desalination processes, especially in remote and arid regions. The optimum combination of RES and RO process has some complexity due to the uncertainty of power supplier in addition to non-linearity of other variables. Bourouni et al. (2011) used GA to integrate all parameters involved and generated several feasible hybrid systems with the objective of minimising the total operating and capital cost of water production.

Park et al. (2012) used GA to correlate key operating parameters and RO permeability statistically. The model developed was used to predict and analyse the performance of a large pilot-scale RO seawater desalination system (1000 m³/day). They obtained a very good match between the model prediction and experimental data. Interestingly, the model was able to analyse the RO system performance even under unsteady conditions.

8.4 GENETIC ALGORITHM OPTIMISATION OF SEVERAL INDUSTRIAL WASTEWATER TREATMENT PROCESSES

GA has been used in several industrial wastewater treatment processes to optimise the operation, reduce total energy consumption, reduce pollutant concentration, and reduce the total operation cost.

Activated sludge wastewater treatment processes are considered as the prominent biological treatment methods for removing organic compounds and ammonium from wastewater. Holenda et al. (2007) applied GA in an aerated wastewater treatment plant using activated sludge to minimise both the pollution load and the operational cost. The activated sludge treatment process included two alternative aerobic and anoxic conditions required for the removal of nitrogen and organic compounds and was achieved by switching the aeration sequentially on and off. The objective was to optimise the aeration period by predicting the number of cycles and the length of the aerated and non-aerated periods. The GA approach offered an optimised solution by reducing both the pollution load and the energy consumption up to 10% compared to traditional control strategies.

Iqbal and Guria (2009) used a binary coded elitist non-dominated sorting genetic algorithm to carry out a multi-objective optimisation for a domestic wastewater treatment plant. NSGA was mainly used to solve multi-objective optimisation problems, which is characterised by selecting the best individuals from the combined

pool of parents and children using both crossover and mutation of the parents, and these become the parent of the next generation based on the concept of elitism (Deb, 2002). Firstly, the kinetic parameters of the activated sludge model were optimised in a single-objective function optimisation problem based on experimental data. Secondly, the multi-objective optimisation problem, with three objective functions of maximising the influent flow rate of wastewater, minimising the exit effluent concentration, and minimising the operating cost, was solved.

An integrated neural network (NN) dynamic model with GA was developed by Fang et al. (2010) to simulate the performance of a complex biological full-scale wastewater treatment plant with considerable influent fluctuations. The NN model was used to link the input and output variables, while the GA method was used to optimise the network weight vectors. The integrated model was able to accurately simulate the five-month performance of a wastewater treatment plant under disturbance in influent concentrations.

Madaeni and Kurdian (2011) developed a simulation model for a microfiltration disinfection process of municipal effluent reuse using a fuzzy inference system. The model was used to predict the water flux and the removal of infectious bovine respiratory (IBR) and foot-and-mouth disease (FMD) viruses from water under different operating conditions. The GA technique was used to carry out parameter optimisation of all parameters involved in the fuzzy system. The model predictions and the observational data of water flux and virus concentration were found to be very close.

GA was also used by Okhovat and Mousavi (2012) to develop a model in a nanofiltration (NF) pilot-scale system in order to predict the removal of arsenic (As), chromium (Cr), and cadmium (Cd) ions, as functions of transmembrane pressure and feed concentration of contaminants. The study developed three empirical models, which were validated against experimental data collected from the NF process.

Oil-polluted wastewater is produced from several industries including oil refineries, petrochemical industries, and metal processing industries. Shokrkar et al. (2012) used GA to predict the permeation flux of microfiltration membranes used to treat oily wastewater. The crossflow velocity, filtration time, oil concentration, transmembrane pressure, and temperature were considered as the input parameters. The model prediction was found to be within 5% of the observational data.

The permeation flux and fouling resistance of commercially polyacrylonitrile (PAN) ultrafiltration (UF) membranes for treating oily wastewaters of the Tehran refinery were predicted and optimised using artificial neural networks (ANNs) and GA by Soleimani et al. (2013). A multi-objective function was used to simultaneously minimise the fouling resistance and maximise the water flux at steady state conditions by optimising the transmembrane pressure, feed flow rate, and pH.

Badrnezhad and Mirza (2014) employed the combination of artificial neural networks and GA to accurately model and optimise the permeate flux of batch-scale crossflow ultrafiltration membrane unit for treating the oily wastewater of the Tehran refinery. The input model parameters were considered as crossflow velocity, transmembrane pressure, filtration time, and operating temperature. The ANN model resulted in a good agreement with observed data collected. The optimal operating conditions for maximum permeate flux were determined by GA.

The NSGA method was used by Lukić et al. (2017) to obtain the optimal operating parameters of microfiltration baker’s yeast using a multi-objective optimisation framework. The transmembrane pressure, suspension concentration, and feed flow rate were selected as control variables to maximise the permeate flux at minimum energy consumption. The optimised control variables resulted in non-dominated maximum solutions of the permeate flux (Pareto-optimal solutions) at a significant reduction of energy consumption of between 44% and 50%.

8.5 REMOVAL OF ORGANIC POLLUTANTS FROM WASTEWATER USING GA BASED OPTIMISATION

Al-Obaidi et al. (2017) used the simple genetic algorithm to carry out an optimisation study for the removal of chlorophenol from wastewater using a single spiral wound RO process with a distributed process model (Model IX, Chapter 5). Two objective functions were selected: one to maximise the chlorophenol rejection at different levels of feed concentration and the other to minimise the applied pressure at an allowable pressure loss to reduce the costs. This was achieved by using optimal values of the operating feed flow rate, pressure, and temperature. The optimisation results yielded a maximum increase of 26.57% of chlorophenol rejection within the allowable constraint of the pressure drop compared to observational data.

As mentioned in earlier chapters, N-nitrosamine compounds and especially N-nitrosodimethylamine (NDMA) are human carcinogens, which can exist in very low concentrations in industrial effluents of many applications (Krauss et al., 2010). Al-Obaidi et al. (2018) used a simple mathematical model of several equations collected from Al-Obaidi et al. models to simulate the performance of a spiral wound RO process for the removal of NDMA from wastewater. The model developed

TABLE 8.1
Summary of GA Applications in Membrane Technology for Wastewater Treatment

Authors	Technique	GA application
Okhovat and Mousavi (2012)	GA	Modelling of NF pilot-scale system to predict the removal of arsenic, chromium, and cadmium from wastewater
Soleimani et al. (2013)	ANNs and GA	Simultaneously optimise the water flux and minimise fouling resistance of UF membrane used to treat oily wastewater
Al-Obaidi et al. (2017)	SGA	Optimise the removal of chlorophenol from wastewater using spiral wound RO process to maintain the process of filtration within a lower operating pressure
Al-Obaidi et al. (2018)	SCGA	Simultaneously optimise the removal of NDMA from wastewater using multi-stage spiral wound RO process and minimise the energy consumption

incorporated SCGA to optimise the NDMA rejection and minimise the energy consumption for several configurations of multi-stage RO process. The operating pressure, flow rate, and temperature were selected as the decision variables. Interestingly, the SCGA provided several optimum solutions for each optimisation problem, and this provided a choice for selecting the most suitable solution.

Table 8.1 summarises the application of GA for optimising the operational parameters of membrane technology including RO-based wastewater treatment process.

8.5.1 CHLOROPHENOL REMOVAL FROM WASTEWATER

Chlorophenol is one of the phenolic compounds which can be found in trace concentrations in effluents of several applications such as petroleum processing and disinfectant, pesticide, herbicide, and plastic production. Al-Obaidi et al. (2017) developed a one-dimensional distributed model (Model IX, Chapter 5) for a spiral wound RO system to predict the performance of chlorophenol removal from wastewater. The model was validated against experimental data and showed good agreement. The model was then used to carry out a multi-objective optimisation using simple genetic algorithm. Both single-objective optimisation and multi-objective optimisation problems were considered. The single-objective optimisation problem was used to maximise chlorophenol rejection, while the multi-objective optimisation was used to maximise chlorophenol rejection and minimise the operating pressure for a set of variable feed concentrations.

8.5.1.1 Optimisation Problem Description and Formulation

Sundaramoorthy et al. (2011) carried out several experiments to evaluate the performance of an RO process for the removal of chlorophenol from wastewater using an individual spiral wound RO pilot-scale plant. This showed a maximum value of 83% for chlorophenol rejection at a feed concentration of $6.226\text{E-}3 \text{ kmol/m}^3$ and a pressure loss of 1.93 atm along the membrane length. SGA was used by Al-Obaidi et al. (2017) to maximise the chlorophenol rejection (Rej) of five cases of feed concentrations ($0.778\text{E-}3$, $1.556\text{E-}3$, $2.335\text{E-}3$, $3.891\text{E-}3$, and $6.226\text{E-}3 \text{ kmol/m}^3$). The decision variables such as the operating pressure ($P_{b(0)}$), flow rate ($F_{b(0)}$) and temperature (T_b) were optimised accordingly. The two optimisation problems are described in Table 8.2.

The upper and lower bounds of the inlet feed flow rate, pressure, and temperature are $<1\text{E-}4\text{--}1\text{E-}3 \text{ m}^3/\text{s}>$, $<4\text{--}24.77 \text{ atm}>$, and $<15\text{--}40 \text{ }^\circ\text{C}>$, respectively. Moreover, the pressure loss (P_{loss}) along the membrane length was constrained to be lower than the membrane specification of 1.38 atm.

For optimisation problem 2, SGA used the following penalty function of the weighted sum fitness assignment to balance both objectives and translate the problem into a single-objective optimisation problem.

$$L = W_1 \times Rej - W_2 \times P_{b(0)} \quad (8.7)$$

W_1 and W_2 are the weighting factors. Note, maximisation of L will maximise rejection and minimise the pressure.

TABLE 8.2
Formulation of Optimisation Problems

Optimisation problem	1		2	
Objective function	Max	Rej	Max Min	Rej $P_{b(0)}$
Optimisation variables	$F_{b(0)}, P_{b(0)}, T_b$		$F_{b(0)}, P_{b(0)}, T_b$	
Subject to:				
Equality constraints				
Process model: $f(z, x(z), x^-(z), u(z), v) = 0$				
Inequality constraints				
	$P_{loss} \leq P_{loss}^d \text{ (1.93 atm)}$			
	$F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U$			
	$F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U$			
	$T_b^L \leq T_b \leq T_b^U$			

8.5.1.2 Genetic Algorithm Parameter Setting

The optimisation problems were solved using SGA. Selected as maximum generation, population size, crossover probability, and mutation probability were 500, 50, 0.6, and 0.1, respectively.

The maximum operating pressure of the membrane used was assumed around 25 atm, while the chlorophenol maximum rejection was assumed to be 1. Therefore, to give equal importance to the two objectives of the optimisation problem 2, W_2 was considered to be $= 1/25 = 0.04$. Table 8.3 shows the effectiveness of selecting W_2 as 0.04 to maintain high chlorophenol rejection at the lowest operating pressure. Any reduction in W_2 can lead to a higher chlorophenol rejection with higher operating pressures. However, no significant impact is noticed for a W_2 with a value of greater than 0.04.

The impact of the generation number with a population size of 50 and a W_2 of value 0.04 on the performance of GA is shown in Table 8.4. Clearly, selecting a larger generation number increases the possibility of identifying an optimal solution due to the larger space for exploring and the ability to evaluate more fitness functions. Fifty generations appear to give the maximum rejection within an acceptable pressure loss inside the membrane.

The impact of the crossover probability, between 0.1 and 0.5, at the recommended parameters of 50 population size, 80 generation number, and 0.04 of W_2 and mutation probability P_m of 0.1 on GA performance is depicted in Table 8.5, which shows an insignificant impact. The variation of the mutation probability also has no considerable effect on GA, as can be shown in Table 8.6 at the fixed crossover probability of 0.4. It is nonetheless reasonable to use a value between 0.01 and 0.02 for the mutation

TABLE 8.3
Impact of the Weighting Factor on the Optimisation Results

W_2	Rej (–)	$Fb_0 \times E4 \text{ (m}^3/\text{s)}$	$Pb_0 \text{ (atm)}$	$Tb \text{ (}^\circ\text{C)}$
0.001	0.95	2.36	21.43	40
0.005	0.92	2.04	11.18	40
0.01	0.90	1.923	7.57	40
0.04	0.90	1.92	7.53	40
0.08	0.90	1.92	7.53	40
0.1	0.90	1.92	7.53	40
0.2	0.90	1.92	7.53	40

(Adapted from Al-Obaidi et al., 2017)

TABLE 8.4
Impact of the Generation Number on GA Results

Generation	Rej (–)	$P_{loss} \text{ (atm)}$	$Fb_0 \times E4 \text{ (m}^3/\text{s)}$	$Pb_0 \text{ (atm)}$	$Tb \text{ (}^\circ\text{C)}$
10	0.87	0.82	1.23	7.53	38.1
20	0.89	0.70	1.07	7.53	40
50	0.90	1.36	1.89	7.53	40
80	0.90	1.38	1.92	7.53	40
100	0.90	1.38	1.92	7.53	40
200	0.90	1.38	1.92	7.53	40

(Adapted from Al-Obaidi et al., 2017)

TABLE 8.5
Impact of the Crossover Probability on GA Results

P_c	Rej (–)	$Fb_0 \times E4 \text{ (m}^3/\text{s)}$	$Pb_0 \text{ (atm)}$	$Tb \text{ (}^\circ\text{C)}$
0.1	0.90	1.92	7.53	40
0.2	0.90	1.92	7.53	40
0.3	0.90	1.92	7.56	40
0.4	0.90	1.92	7.53	40
0.5	0.90	1.92	7.53	40

(Adapted from Al-Obaidi et al., 2017)

TABLE 8.6
Impact of the Mutation Probability on GA Results

P_m	Rej (–)	$P_{loss} \text{ (atm)}$	$Fb_0 \times E4 \text{ (m}^3/\text{s)}$	$Pb_0 \text{ (atm)}$	$Tb \text{ (}^\circ\text{C)}$
0.01	0.90	1.37	1.91	7.53	40
0.02	0.90	1.36	1.89	7.53	40
0.05	0.90	1.38	1.92	7.56	40
0.4	0.90	1.38	1.92	7.53	40
0.5	0.90	1.38	1.92	7.53	40

(Adapted from Al-Obaidi et al., 2017)

probability to maintain a lower pressure drop. The crossover and mutation probabilities have a minor influence on the GA performance for optimisation problem 2.

8.5.1.3 Optimisation Results

The optimisation results of problem 1 for the selected set of feed concentrations and the optimised decision variables are given in Table 8.7. It is clear that GA has generated an optimal chlorophenol rejection at the maximum allowable pressure compared to the observational data of Sundaramoorthy et al. (2011). However, GA has achieved this at the lowest allowed feed flow rate (1E-4 m³/s) to guarantee a lower pressure drop in the membrane channel. This has a positive impact on the water flux, which enhances the permeate concentration. The use of GA has yielded the maximum rejection at the highest temperature for the highest feed concentration compared to other medium and low concentrations.

Table 8.7 shows that the GA achieves the highest possible rejection at medium and low feed concentrations when increasing the operating pressure as a result of increasing the feed concentration. However, the GA has selected the lower temperature bound in these conditions. In contrast, the GA has selected the maximum allowable pressure and temperature to drive the process towards the maximum rejection in the case of the highest feed concentration (Case 1). It can therefore be said that the temperature has a positive impact on the water flux as a result of reducing the viscosity and thermal expansion of the membrane (Thirugnanasambandham et al., 2016) as well as the possibility of increasing the solute diffusion and adsorption to membrane surface, which possibly retards the membrane rejection. Table 8.8 shows the retardation of chlorophenol rejection due to decreasing the temperature for the highest feed concentration (Case 1), and it therefore systematically explains the effect of temperature.

Table 8.9 shows the optimised decision variables for five cases with the feed concentrations obtained by GA. A noticeable difference in chlorophenol rejection can be seen for optimisation problem 2 compared to those obtained by optimisation problem 1. Obviously, balancing the two objectives, under the given constraints on pressure,

TABLE 8.7
Optimisation Results of Optimisation Problem 1

Case	Feed conc. $C_{b(0)}$ $\times 10^3$, kmol/m³	Maximum experimental Rej (*)	Experimental $P_{loss}^d(*)$	GA Rej (–)	GA P_{loss}^d (atm)	Decision variables		
						$Fb_{(0)} \times E4$ (m³/s)	$Pb_{(0)}$ (atm)	T_b (°C)
1	6.226	0.83	1.93	0.98	0.42	1.04	24.77	40
2	3.891	0.77	1.89	0.99	0.39	1.00	21.64	15
3	2.335	0.75	1.84	0.99	0.39	1.00	18.87	15
4	1.556	0.72	1.79	0.99	0.39	1.00	17.48	15
5	0.778	0.66	1.74	0.99	0.39	1.00	16.09	15

* Sundaramoorthy et al., 2011
(Adapted from Al-Obaidi et al., 2017)

TABLE 8.8**The Impact of Temperature (Upper Bound) on Case 1 of Optimisation Problem 1**

Up limit of temperature	GA		Decision variables		
	Rej (–)	P_{loss} (atm)	$Fb_{(0)} \times E4$ (m ³ /s)	$Pb_{(0)}$ (atm)	T_b (°C)
40	0.98	0.42	1.05	24.77	40
39	0.97	0.43	1.06	24.77	39
38	0.96	0.45	1.07	24.77	38
37	0.94	0.46	1.09	24.77	37
36	0.95	0.41	1.0	24.77	15
35	0.95	0.41	1.0	24.77	15
34	0.95	0.41	1.0	24.77	15

(Adapted from Al-Obaidi et al., 2017)

TABLE 8.9**Optimisation Results of Optimisation Problem 2**

Case	Feed conc. $C_{b(0)} \times 10^3$, kmol/m ³	Maximum experimental Rej (*)	Experimental P_{loss}^d (*)	GA Rej (–)	Decision variables		
					$Fb_{(0)} \times E4$ (m ³ /s)	$Pb_{(0)}$ (atm)	T_b (°C)
1	6.226	0.83	1.93	0.90	1.922	7.53	40
2	3.891	0.77	1.89	0.89	1.931	7.47	40
3	2.335	0.75	1.84	0.88	1.939	7.45	40
4	1.556	0.72	1.79	0.87	1.942	7.41	40
5	0.778	0.66	1.74	0.84	1.945	7.32	40

GA $P_{\text{loss}} = 1.38$ (atm). * Sundaramoorthy et al., 2011

(Adapted from Al-Obaidi et al., 2017)

resulted in the process to select the lowest possible pressure and maximise the rejection as much as possible. For a single-objective optimisation (Table 8.7), the choice of higher pressure (within constraints) led to a higher rejection (almost 99%). Higher pressure leads to an economic penalty but at the highest fulfilment of environmental requirement. On the other hand, a lower pressure is favourable economically but not environmentally. The choice of the weighting factors given in Eq. (8.7) are therefore different for different requirements.

For optimisation problem 2, GA has selected the highest allowed temperature to compensate for the hidden impact of pressure after pushing the process towards the lowest pressure. Again, the effect of temperature is straightforward as shown in Table 8.10 for the highest feed concentration (Case 1), where chlorophenol rejection increases when the temperature increases.

TABLE 8.10
The Effect of Temperature (Upper Limit) on the Optimisation Problem 2

Up limit of temperature	Rej (–)	Decision variables		
		$Fb_{(0)} \times E4 \text{ (m}^3/\text{s)}$	$Pb_{(0)} \text{ (atm)}$	$T_b \text{ (}^\circ\text{C)}$
0	0.90	1.922	7.53	40
39	0.89	1.919	7.53	39
38	0.88	1.917	7.53	38
37	0.87	1.914	7.53	37
36	0.86	1.911	7.53	36
35	0.84	1.907	7.53	35
34	0.83	1.903	7.53	34

GA $P_{loss} = 1.38 \text{ (atm)}$
(Adapted from Al-Obaidi et al., 2017)

8.5.2 N-NITROSODIMETHYLAMINE (NDMA) REMOVAL FROM WASTEWATER

The existence of micropollutants such as N-nitrosamine (hydrophilic compound), even at low concentrations in drinking and reused water resources, continues to pose a considerable threat to the environment. N-nitrosamine compounds and especially N-nitrosodimethylamine (NDMA) are classified as highly toxicological and carcinogenic compounds that can be formed as by-products of complicated reactions in the effluents of several facilities. RO processes, however, have been successfully used to abate organic compounds from wastewater. The efficiency for eliminating NDMA from wastewater typically ranges from 40% to 70%. NDMA has a low molecular size in addition to uncharged properties, which enhances permeation through the RO membrane (Steinle-Darling et al., 2007; Plumlee et al., 2008; Krauss et al., 2010). The recent experimental work of Fujioka et al. (2018) confirmed the possibility of a 92% rejection of NDMA. However, this is achieved at the expense of a very low water transport parameter and a permeate recovery rate. Al-Obaidi et al. (2018) explored and assessed the performance of several configurations of multi-stage RO processes, including the utilisation of permeate reprocessing design for the removal of NDMA from wastewater. Therefore, an analytical model was developed for this purpose and validated against the experimental data by Fujioka et al. (2014). The model was augmented with the species conserving genetic algorithm to minimise NDMA rejection, maximise water recovery rate, and minimise total energy consumption.

8.5.2.1 Description of Permeate Reprocessing Multi-Stage RO Process

Figure 8.7 shows schematic diagrams of five configurations (A to E) for the investigation of permeate reprocessing of a multi-stage RO process. Specifically, six pressure vessels connected in different arrangements of stages were selected for each configuration where each pressure vessel holds three elements connected in series of spiral wound RO membrane type BW30–400 of 37.2 m² produced by Dow/FilmTec.

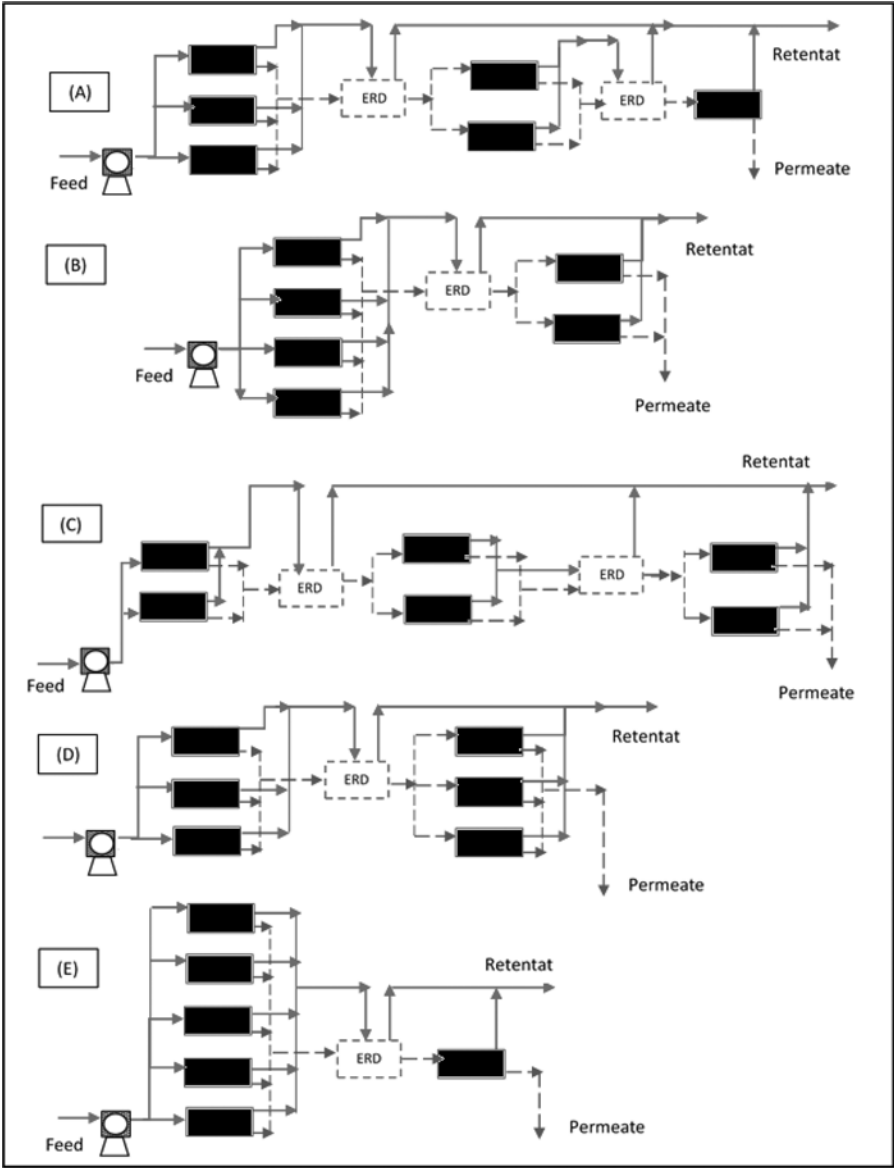


FIGURE 8.7 Schematics of various configurations of multi-stage permeate reprocessing RO system.

(Adapted from Al-Obaidi et al., 2018)

The permeate reprocessing design is essentially achieved by blending the permeate of stage 1 to form the feed stream of the next stage, and so on. An energy recovery device (ERD) was used in the proposed configurations to transfer the potential energy from the high-pressure streams to the low-pressure streams.

8.5.2.2 Optimisation Problem Description and Formulation

The simultaneous maximisation of NDMA rejection ($Rej_{(NDMA)}$) and minimisation of energy consumption (EC) were selected to form the multi-objective optimisation problem for the proposed configuration of Figure 8.7 to be solved using the SCGA. The inlet feed concentration ($Cf_{(plant)}$) of NDMA was 1000 ng/L. The lower and upper recommended limits of the feed flow rate of the whole plant ($Q_{f(plant)}$) and each membrane (Q_f), operating pressure ($P_{(plant)}$), and membrane pressure ($P_{f(in)}$) and operating temperature ($T_{(plant)}$), and a maximum pressure drop of 0.987 atm were set as constraints for the optimisation problem. The maximum and minimum limits of the plant operating conditions are mainly dependent on the number of parallel pressure vessels in the first stage. However, the operating conditions of each membrane were within the manufacturers' specification.

The mathematical description of the multi-objective optimisation problem is as follows:

$$\begin{array}{ll}
 \text{Max} & Rej_{(NDMA)} \\
 \text{Min} & EC \\
 & Q_{f(plant)}, P_{f(plant)}, T_{(plant)}
 \end{array}$$

Subject to:

Equality constraints:

Process model $g(z, u, v) = 0$

Inequality constraints of the plant:

$$\begin{aligned}
 & Q_{f(plant)}^L \leq Q_{f(plant)} \leq Q_{f(plant)}^U \\
 (10 \text{ atm}) & P_{f(plant)}^L \leq P_{f(plant)} \leq P_{f(plant)}^U \quad (40.463 \text{ atm}) \\
 (20 \text{ }^\circ\text{C}) & T_{(plant)}^L \leq T_{(plant)} \leq T_{(plant)}^U \quad (45 \text{ }^\circ\text{C})
 \end{aligned}$$

Inequality constraints of the element:

$$\begin{aligned}
 (1.008\text{E-}3 \text{ m}^3/\text{s}) & Q_f^L \leq Q_f \leq Q_f^U \quad (5.363\text{E-}3 \text{ m}^3/\text{s}) \\
 (10 \text{ atm}) & P_{f(in)}^L \leq P_{f(in)} \leq P_{f(in)}^U \quad (40.463 \text{ atm}) \\
 (20 \text{ }^\circ\text{C}) & T^L \leq T \leq T^U \quad (45 \text{ }^\circ\text{C}) \\
 & \Delta P_{drop} \leq 0.987
 \end{aligned}$$

8.5.2.3 Optimisation Results

The optimisation results of the proposed configurations A to E as shown in Figure 8.7 are subject to the same inlet feed concentration of 1000 ng/L of NDMA and are given in Table 8.11. The GA has introduced four and three optimal solutions for configurations A and D, respectively, compared to only two solutions for other configurations (B, C, and E). The design of RO membranes used in each configuration might interpret the number of optimal solutions of GA.

Table 8.11 shows a different number of optimal solutions that can be provided for the tested configurations A, B, C, D, and E. This is originally related to the methodology used of SCGA that selected the optimal solutions for each case. However, the operator has an open opportunity to select the highly recommended optimal solution based on the existing conditions. These results include the optimal operating conditions corresponding to the maximum NDMA rejection and minimum energy consumption obtained for each layout tested. The best optimum solution is highlighted in bold in Table 8.11.

Optimisation results show the possibility of a high NDMA removal of the permeate reprocessing design compared to the rejection (between 40% and 70%), as mentioned in the literature. Solution A1 is close to that obtained by Fujioka et al. (2018). However, solution A2 is the best one, while solution E2 is the worst one in terms of NDMA rejection.

Only configuration C appears to yield a high permeate recovery rate at a high NDMA rejection compared to other configurations. Indeed, the recovery of configurations A and E are the worst ones. This is possibly caused by the presence of only one pressure vessel in the last stage. Configuration E has the lowest recovery in comparison to configuration A. The blending of permeate streams of five pressure vessels in configuration E (compared to two pressure vessels in configuration A) causes a higher feed flow rate in the final module of configuration E. This increases the bulk velocity inside the last module, and this leads to a lower recovery rate. Increasing feed velocity inside the membrane module would reduce the residence

TABLE 8.11
Optimisation Results of Configurations A to E (Fresh Feed Concentration:
 $C_{f(plant)}=1000$ ng/L)

Configuration	Solutions	The decision variables			Optimisation results			
		$Q_{f(plant)}$ (m ³ /h)	$P_{f(plant)}$ (atm)	$T_{f(plant)}$ (°C)	$Rej_{(NDMA)}(-)$	$Rec_{(plant)}(-)$	$C_{p(plant)} \times 10^8$ (kg/m ³)	$EC(kWh/m^3)$
A	1	30.35	27.50	20.00	92.17	20.98	7.38	3.37
	2	43.20	32.20	22.30	94.60	17.20	5.40	4.78
	3	46.69	30.20	27.40	94.22	17.50	5.78	4.42
	4	42.66	27.39	29.71	93.25	18.18	6.75	3.85
B	1	59.62	31.28	20.00	87.01	27.32	13.00	2.96
	2	76.61	26.95	20.65	87.47	18.16	12.50	3.12
C	1	38.59	38.45	22.68	90.21	50.15	9.79	1.96
	2	38.63	35.96	20.60	90.17	44.39	9.83	1.96
D	1	57.92	36.24	20.00	82.24	49.55	17.80	1.78
	2	57.38	40.17	20.06	82.00	55.93	18.00	1.87
	3	49.50	34.19	20.02	80.25	54.97	19.80	1.60
E	1	59.33	13.64	20.00	79.07	5.34	20.90	4.77
	2	50.58	13.22	20.54	77.93	6.20	22.10	4.22

(Adapted from Al-Obaidi et al., 2018)

time of the fluid inside the module that would reduce the water permeation through the membrane pores and therefore reduces the water recovery. Solution D2 is the best and E1 is the worst in terms of permeate recovery. However, solution D3 is the best in terms of energy consumption compared to solution A2 as being the worst. Overall, solution C1 represents the best configuration based on three performance indicators of rejection, recovery, and energy consumption, while configuration E yields the lowest performance

8.6 CONCLUSIONS

This chapter has provided the state of the art on the use of genetic algorithms (GA) for optimising the performance of membrane-based seawater desalination and wastewater treatment plants, including more specifically RO processes for the removal of highly toxic organic compounds from wastewater. GA provides one of the best tools for optimising the performance of membrane technologies, including more specifically RO processes. One of the most important advantages of using GA is its ability to provide several global and local solutions for a specified multi-objective problem at the end of each iteration, compared to a solitary solution. The chapter has also highlighted the latest research on how GA has been successfully used to optimise the removal of phenolic and N-nitrosamine compounds from wastewater using RO process.

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9 Recent Advances of Reverse Osmosis Design for Wastewater Treatment

9.1 INTRODUCTION

RO processes are generally energy intensive. They are configured in different layouts including single-stage, two-stage, multi-stage, single-pass, and two-pass systems. The need to improve such processes for the removal of the persistent and highly toxic compounds continues to be a challenge. Improved designs of multi-stage RO process with appropriate optimisations can provide economical and better solutions for removing such harmful compounds from wastewater at minimum energy consumption.

This chapter discusses recent advances in the design of RO processes using model-based optimisation techniques for the removal of highly toxic compounds from wastewater and with improved rejection of pollutants, water recovery, and energy efficiency. This can be achieved by optimising membrane design and operating parameters with permeate and retentate recycling in an integrated multi-pass design of RO process.

9.2 ADVANCED DESIGN OF MULTI-STAGE RO PROCESS FOR THE REMOVAL OF N-NITROSAMINE COMPOUNDS FROM WASTEWATER

N-nitrosamine organic compounds of N-nitrosodimethylamine-D6 (NDMA), N-nitrosomethylethylamine-D3 (NMEA), and N-nitrosopyrrolidine-D8 (NPYR) are some of the highly toxic compounds of the N-nitrosamine family, which have been specifically detected in chlorinated water and considered as probable human carcinogens. The removal of these compounds, especially NDMA from water, is becoming a real challenge due to their low molecular weights and high hydrophilic properties. This section shows a new advanced design of a multi-stage RO process proposed by Al-Obaidi et al. (2018a) to remove the selected compounds of N-nitrosamine from wastewater. This also includes a thorough study to assess the impact of the operating parameters of pressure, feed flow rate, and temperature on the RO process performance of the N-nitrosamine rejection, recovery rate, and total energy consumption. Al-Obaidi et al. (2018a) carried out a simulation analysis on a pilot-scale crossflow

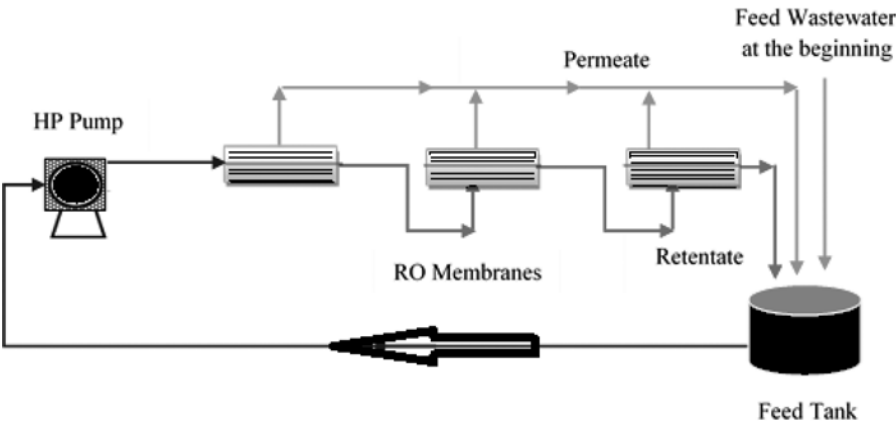


FIGURE 9.1 Schematic diagram of the pilot-scale plant used by Fujioka et al. (2014). (Adapted from Fujioka et al., 2014)

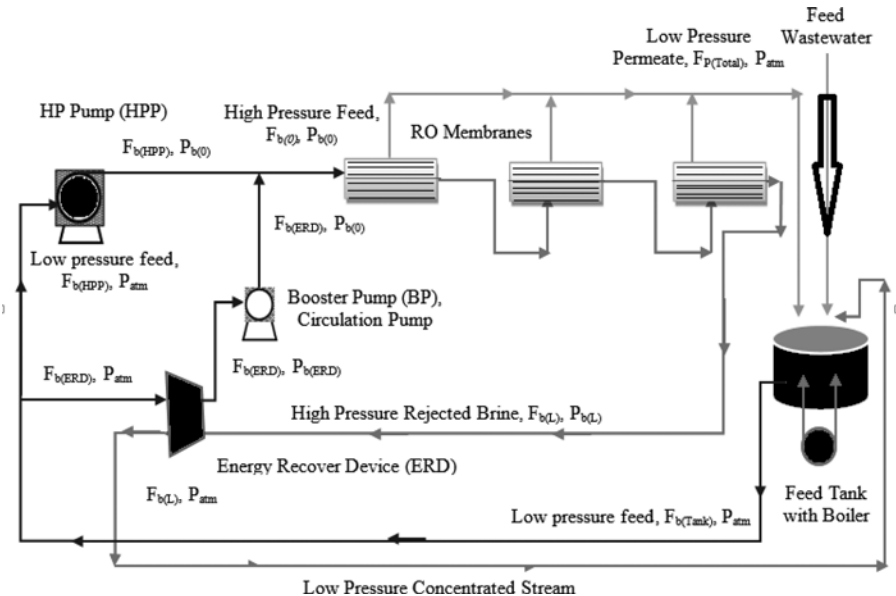


FIGURE 9.2 Schematic diagram of a conventional RO pilot-scale plant. (Adapted from Al-Obaidi et al., 2018a)

RO filtration system (Figure 9.1) used by Fujioka et al. (2014) on the configuration shown in Figure 9.2 using the Model VI described in Chapter 5.

9.3.1 DESCRIPTION OF THE MULTI-STAGE RO PROCESS

The proposed RO configuration by Al-Obaidi et al. (2018a) is schematically presented in Figure 9.2. This shows three 4" glass-fibre pressure vessels, where

each pressure vessel holds one membrane (make: Hydranautics, Oceanside, CA, USA). The system includes a high-pressure pump (HPP), a booster pump (BP), an energy recovery device (ERD), and the feed tank boiler (electric). This configuration is basically the same as that considered by Fujioka et al. (2014), which is shown in Figure 9.1 but without an ERD. The electric boiler is included in the set-up to investigate the impact of feed temperature on the process operation. This is done by running the process at a reference temperature of 20 °C followed by boiling the feed tank from 20 to 22 °C in one hour, and running the process in a step change of 2 °C at the new temperature of 22 °C, and so on until the process temperature is raised to 44 °C. The operation was carried out at a fixed feed concentration where the retentate and permeate are recycled back to the feed tank. The outflow of the feed tank was split into two streams; one feeding the HPP at the atmospheric pressure and the other feeding the ERD. The high-pressure rejected brine stream discharged from the last module transfers the surplus energy to the low-pressure incoming feed stream at the ERD. This helps reduce the process energy consumption. The outflow feed stream from the ERD is further pressurised using a booster pump. Finally, the outflows of the HPP and BP are combined to form the feed stream to the RO modules at the desired operating pressure. Al-Obaidi et al. (2018a) used the contaminant rejection and total recovery rate as the process performance indicators. They also calculated the specific energy consumption of the proposed configuration and compared it to the one presented by Fujioka et al. (2014).

9.3.2 MODEL XV (AL-OBaidi ET AL. (2018A))

The one-dimensional model developed by Al-Obaidi et al. (2017a) (Model XIII, Chapter 5) was used here to estimate the process performance. However, several new equations were added to this model, which identified a new version of the model. In this respect, the empirical expression of Senthilmurugan et al. (2005) was used to estimate the mass transfer coefficient along the feed channel (x-axis), as follows:

$$k_{(x)} = 0.753 \left(\frac{K}{2-K} \right)^{0.5} \left(\frac{D_{b(x)}}{t_f} \right) \left(\frac{\mu_{b(x)} \rho_{b(x)}}{D_{b(x)}} \right)^{0.1666} \left(\frac{2 t_f^2 U_{b(x)}}{D_{b(x)} \Delta L} \right)^{0.5} \quad (9.1)$$

Also, the impact of feed temperature on water and solute permeability coefficients were included using the proposed expression of Sarkar et al. (2008):

$$L_{p(T_b+273.15)} = L_{p(T_o+273.15)} \frac{\mu_{b(T_o+273.15)}}{\mu_{b(T_b+273.15)}} \quad (9.2)$$

$$B_{s(T_b+273.15)} = B_{s(T_o+273.15)} \frac{T_b + 273.15}{T_o + 273.15} \frac{\mu_{b(T_o+273.15)}}{\mu_{b(T_b+273.15)}} \quad (9.3)$$

T_o represents the reference temperature of 20 °C. Al-Obaidi et al. (2018a) aimed to evaluate the energy consumption of the process due to its important contribution to the total filtration cost. Therefore, the calculation of specific energy consumption based on the proposed expression of Qi et al. (2012) was considered for both the proposed configuration of Fujioka et al. (2014) (Figure 9.1), expressed as E1 (based

on the use of only a high-pressure pump) and the new configuration (Figure 9.2) as proposed by Al-Obaidi et al. (2018a) expressed as E2 (based on the use of a high-pressure pump, booster pump, and ERD).

$$E1 = \frac{\left((P_{b(0)} 101325) F_{b(0)} \right)}{\frac{F_{p(Total)} \varepsilon_{pump}}{36E5}} \quad (9.4)$$

$$E2 = \frac{\left((P_{b(0)} 101325) F_{b(0)} \right)}{\frac{F_{p(Total)} \varepsilon_{pump}}{36E5}} - \frac{(P_{b(L)} 101325) F_{b(L)} \varepsilon_{ERD}}{\frac{F_{p(Total)}}{36E5}} \quad (9.5)$$

The outlet pressure of the ERD ($P_{b(ERD)}$) was calculated by Eq. (9.6) based on the outlet pressure of membrane modules $P_{b(L)}$.

$$\varepsilon_{ERD} = \frac{P_{b(ERD)}}{P_{b(L)}} \quad (9.6)$$

Eq. (9.7) was used to calculate the heat supplied Q (j/s) by the boiler based on the reference temperature of the feed tank $T_{ref} = 20$ °C.

$$\frac{d(T_{Tank} - T_{Ref})}{dt} = \frac{Q}{\rho C_p V} \quad (9.7)$$

ρ , C_p and V represent the density of water (kg/m³), specific heat capacity of water (j/kgK), and volume of feed tank (m³), respectively. Therefore, Eqs. (9.8) and (9.9) were used to calculate the boiler energy consumption $E3$ (kWh/m³ of permeate) and the total energy consumption $E4$ (kWh/ m³ of permeate) considering the energy consumption of the HPP and boiler in addition to the gain in energy due to using the ERD.

$$E3 = \frac{\left(\frac{Q}{F_{p(Total)}} \right)}{36E5} \quad (9.8)$$

$$E4 = E2 + E3 \quad (9.9)$$

9.3.3 SENSITIVITY ANALYSIS OF THE OPERATING PARAMETERS

The impact of the operating pressure variation at the fixed inlet feed flow rate and operating temperature of 2.43E-3 m³/s and 20 °C, respectively, on the N-nitrosamine rejection, total recovery, and energy consumption for the RO configurations of Figure 9.1 and 9.2 is addressed in the following section. Three inlet feed concentrations of N-nitrosamine solutes (similar to those used by Fujioka et al., 2014) are

considered and are given in Table 9.1. The specifications of the spiral wound membrane module are given in Table 9.2.

Figure 9.3 illustrates the impact of the operating pressure on the N-nitrosamine rejection for all N-nitrosamine feed concentrations. Increasing the pressure results in a higher permeate flux and a lower concentration at the permeate channel. An increase of around 30% (from 0.60 to 0.78) is noticed for NDMA, while an increase of 9.57% (from 0.87 to 0.95) is noticed for the NMEA rejection and an increase of 4.55% (from 0.936 to 0.978) is noticed for the NPYR rejection.

Figure 9.4 shows the variation of the specific energy consumption and the total recovery with the pressure for the RO configurations shown in Figures 9.1 and 9.2. It can be seen that increasing the operating pressure results in a decreasing energy consumption for the configuration with only HPP (Figure 9.1) and a further reduction of energy consumption caused by increasing the pump efficiency from 80% to 85% and then to 90%. This would specifically confirm that a significant energy consumption reduction could be achieved by increasing the pump efficiency. These findings

TABLE 9.1
Physical and Transport Parameters of NDMA, NMEA, and NPYR

Name	Molecular weight (g/mol)	Inlet feed concentration, $C_{s(0)} \times 10^9$ (kmol/m ³)	Solute permeability coefficient, B_s (m/s) at 20 °C	Reflection coefficient, σ (dimensionless)
NDMA	74.1	3.376	5.35×10^{-6}	0.953
NMEA	88.1	2.839	1.14×10^{-6}	0.958
NPYR	100.1	2.499	5.12×10^{-7}	0.973

(Adapted from Al-Obaidi et al., 2018a)

TABLE 9.2
Specifications of the Composite Polyamide Spiral Wound Membrane Element

Make	Hydranautics, Oceanside, CA, USA
Membrane type	ESPA2-4040
Feed spacer thickness t_f (m)	6.6×10^{-4}
Membrane sheet active area (m ²)	7.9
Membrane sheet length L and width W (m)	0.9 and 8.78
Characteristics length of spacer ϕ_L (m)	0.006
Maximum applied pressure (atm, bar)	41.06, 41.6
Maximum operating temperature (°C)	45
Salt rejection (dimensionless)	% (99.4% minimum)

(Adapted from Al-Obaidi et al., 2018a)

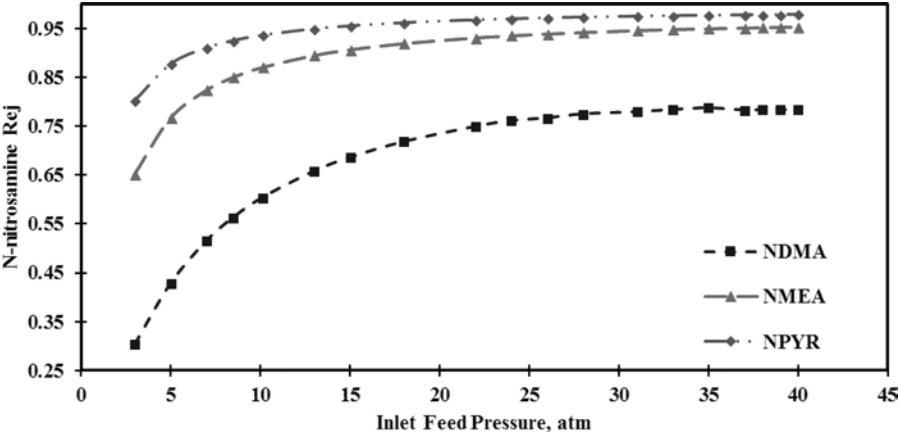


FIGURE 9.3 N-nitrosamine rejection vs inlet feed pressure (inlet feed conditions of $2.43\text{E-}3\text{ m}^3/\text{s}$ and $20\text{ }^\circ\text{C}$).

(Adapted from Al-Obaidi et al., 2018a)

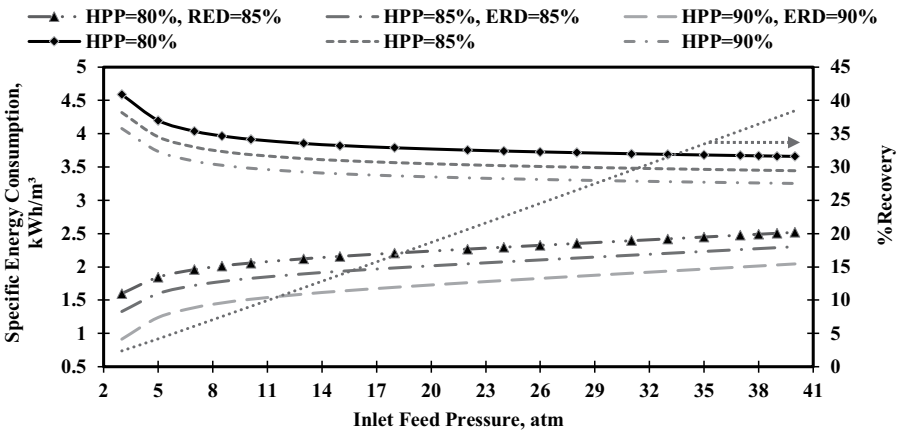


FIGURE 9.4 Specific energy consumption of two types of RO pilot plants without and with ERD (Figures 9.1 and 9.2) and total recovery versus inlet feed pressure at inlet feed conditions of $2.43\text{E-}3\text{ m}^3/\text{s}$ and $20\text{ }^\circ\text{C}$.

(Adapted from Al-Obaidi et al., 2018a)

are in line with those of Du et al. (2014). However, the addition of an ERD, as shown in Figure 9.2, reduces the energy consumption significantly (47% at a pressure of 10.1 atm and 31% at 40 atm) compared to cases with only HPP. This is due to the fact that the rejected (retentate) stream holds a high amount of hydraulic energy, which is extracted and reused to pressurise the feed stream via the ERD. Furthermore, increasing the operating pressure increases the recovery rate (Figure 9.4) as well

as increases the specific energy consumption for the configuration with an ERD. However, the increased efficiency of ERD reduces the energy consumption. Another interesting point to be noticed is that the pressure influences the energy consumption more significantly at low pressures than at high ones. Figure 9.4 depicts the increase of energy consumption as a result of increasing water recovery for the ERD system.

The impact of feed flow rate on N-nitrosamine rejection, recovery rate, and energy consumption at fixed values of inlet feed pressure and temperature is shown in Figure 9.5. The fixed operating pressure and temperature were 10.1 atm and 20 °C, respectively.

The expectation is that a rise of the feed flow rate improves the rejection due to mitigating the concentration polarisation. However, increasing the feed flow rate would increase the friction, which increases the pressure loss at the feed channel. This then reduces the water flux as well as lowers the osmotic pressure and concentration polarisation. It can therefore slightly reduce the rejection. This explains why insignificant changes in N-nitrosamine rejection of NMEA, NPYR, and NDMA were noticed as a result of increasing the feed flow rate. Abbas (2005) reported similar findings.

Figure 9.6 shows that the specific energy consumption increases when the inlet feed flow rate at fixed pressure and temperature is increased. However, the opposite trend is observed for the recovery rate. The inclusion of an ERD reduces the energy consumption further compared to the cases with a HPP only (Figure 9.6). Al-Obaidi et al. (2018a) observed that a low inlet feed flow rate leads to a higher recovery rate, due to the low pressure drop in the system.

The impact of the operating temperature on N-nitrosamine rejection, recovery rate, and energy consumption at fixed values of inlet feed flow rate and pressure

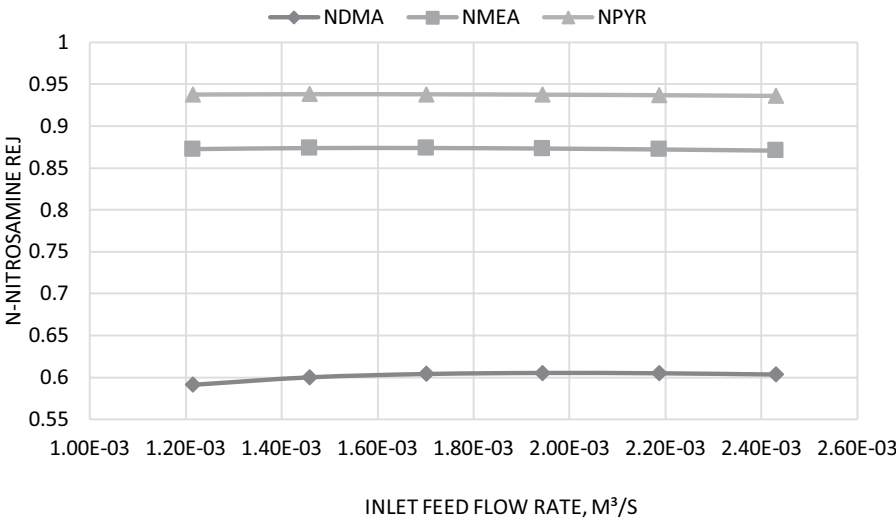


FIGURE 9.5 N-nitrosamine rejection vs inlet feed flow rate at inlet feed conditions of 10.1 atm and 20 °C.

(Adapted from Al-Obaidi et al., 2018a)

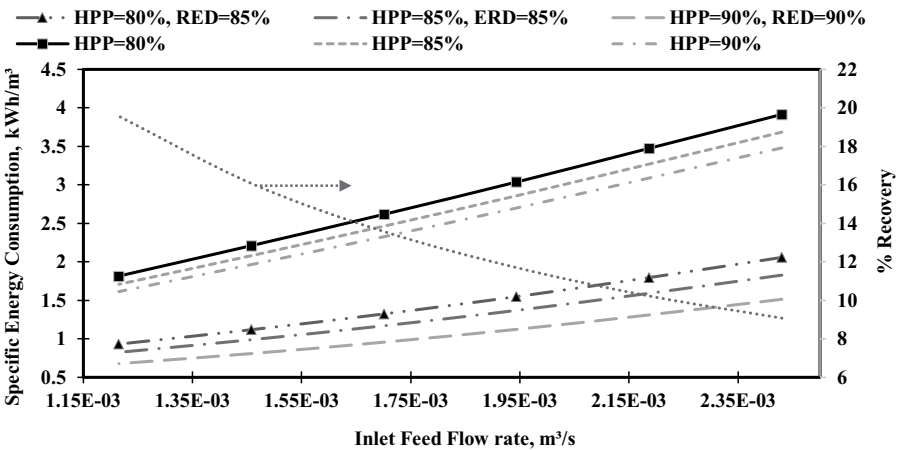


FIGURE 9.6 Specific energy consumption versus inlet feed flow rate at inlet feed conditions of 10.1 atm and 20 °C.

(Adapted from Al-Obaidi et al., 2018a)

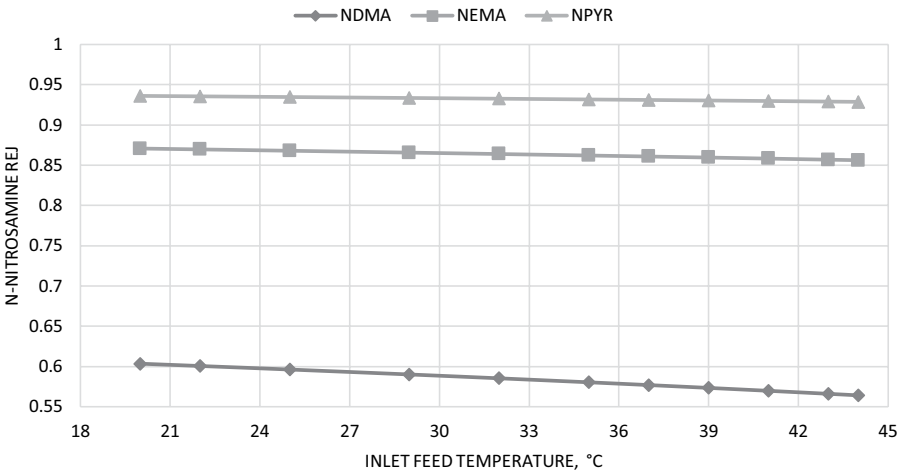


FIGURE 9.7 N-nitrosamine rejection vs inlet feed temperature at inlet feed conditions of 2.43E-3 m³/s and 10.1 atm.

(Adapted from Al-Obaidi et al., 2018a)

was investigated for every 2 °C rise in the feed temperature (the reference feed temperature was 20 °C). Firstly, a slight decrease of N-nitrosamine compound rejection and a noticeable increase of recovery rate were noticed as a result of increasing the operating temperature (Figures 9.7 and 9.8). The N-nitrosamine results are in line with the ones reported by Fujioka (2014). They noted an

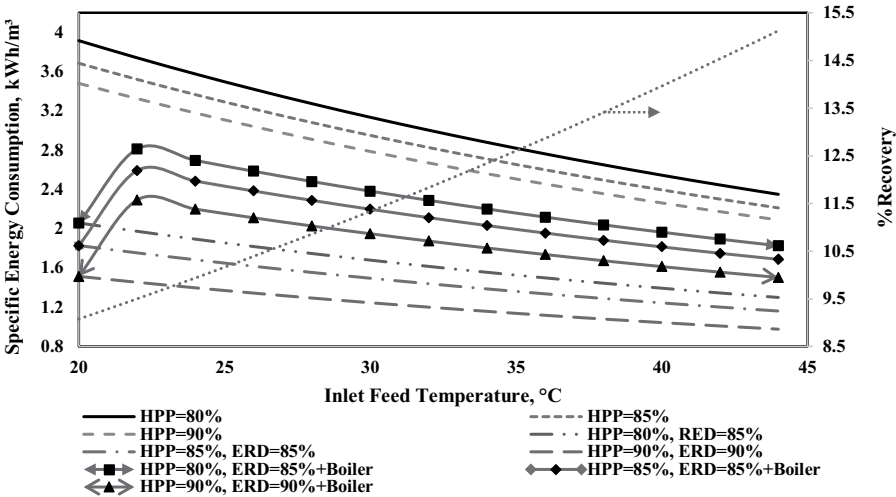


FIGURE 9.8 Specific energy consumption of two types of RO pilot plants with and without ERD, and ERD with boiler and total recovery versus inlet feed temperature at inlet conditions of 2.43E-3 m/s and 10.1 atm.

(Adapted from Al-Obaidi et al., 2018a)

increasing membrane pore size as well as an elevated solute transport parameter as a response to increasing the temperature. In other words, the increase causes an increase of the solute flux, which slightly retards the solute rejection. Reductions of 6.5% (from 0.6 to 0.56), 1.7% (from 0.87 to 0.85), and 0.79% (from 0.936 to 0.926) were registered for NDMA, NMEA, and NPYR, respectively (Figure 9.7). This corresponds to an increase of around 67% in the permeate recovery due to the increasing temperature from 20 to 44 °C. Increasing the temperature would increase the energy consumption by around 28% and 32% for the proposed configurations with and without ERD, respectively, as given in Figure 9.8. It can therefore be said that the temperature has a significant role in reducing the energy consumption due to the lifting up of the recovery rate. Jiang et al. (2015) confirmed that the temperature has an obvious impact on the process performance including rejection, water recovery, and energy consumption. It is important to mention that the simulation has not considered the contribution of the boiler energy, which is essential for increasing the feed temperature from 20 to 44 °C. Al-Obaidi et al. (2018a) assumed that a 1-hour operating time was sufficient for increasing the temperature of the feed tank to the next level. The total heat supplied Q (measured in watts) was estimated using Eq. (9.7) without any heat loss. Undoubtedly, the inclusion of the boiler energy consumption increases the total energy consumption of the whole system as illustrated in Figure 9.8. Simulation results showed that the energy consumption with the addition of the boiler was still lower than the energy consumption in the HPP mode. Moreover, the total energy consumption with the ERD shows a reasonable increase after increasing the temperature from 20 to 22 °C due to the addition of boiler energy consumption (Figure 9.8). However, a

progressive decrease of energy consumption was noticed after increasing the tank temperature from 22 to 44 °C. The reason behind this is that a significant increase of water flux and permeate flowrate was noticed when the feed temperature was increased. Consequently, the total energy consumptions (E_1 , E_2 , E_3 , E_4) will be reduced due to a rise of the total permeate flow rate ($F_{p(Total)}$) as given in Eqs. (9.4), (9.5), (9.8), and (9.9).

The simulation results presented earlier can be summarised as follows:

- Increasing the feed pressure at constant feed flow rate and temperature would significantly improve N-nitrosamine rejection and total recovery.
- Increasing the feed temperature at constant pressure and flow rate or increasing flow rate at constant pressure and temperature reduces N-nitrosamine rejection.
- An increment in the feed flow rate has a passive effect on the recovery rate.
- An increase in the feed pressure at constant feed flow rate and temperature or an increase of the feed flow rate at constant feed pressure and temperature causes an adverse impact on the energy consumption of the ERD and HPP configuration.
- An increase in the feed temperature at constant pressure and flow rate increases the energy consumption but within acceptable levels, in spite of the inclusion of the consumed energy of the boiler (source of heat).
- The combination of ERD and HPP (Figure 9.2) results in a higher reduction of the energy consumption compared to the configuration of Fujioka et al. (2014) based on the use of only the HPP mode (Figure 9.1).

9.3.4 OPTIMISATION OF A MULTI-STAGE RO PROCESS WITH ERD

Fujioka et al. (2014) achieved a maximum NDMA rejection between 40% and 61% for the three membranes connected in series, as shown in Figure 9.1. Krauss et al. (2010) confirmed a range between 40% and 70% for the rejection of NDMA from wastewater using an RO process.

Al-Obaidi et al. (2018a) carried out optimisation of the multi-stage RO process presented in Figures 9.1 and 9.2. The optimisation problem was formulated to maximise the rejection of N-nitrosamine and minimise the total energy consumption while optimising the operating conditions. The lowest rejections of N-nitrosamine compounds obtained by Fujioka et al. (2014) were set as the lowest accepted values in the optimisation problem. Two optimisation problems were considered by Al-Obaidi et al. (2018a) and are described in the next sections.

9.3.4.1 Optimisation Problem 1 (OP1)

- Given: inlet feed conditions, module specifications.
- Optimise: the inlet feed pressure, flow rate, and temperature.
- Maximise: NDMA rejection.
- Subject to: equality and inequality constraints of process model and linear bounds of optimisation variables, respectively.

Therefore, the mathematical expression of OP1 is as follows;

$$\text{Max} \quad Rej$$

$$F_{b(0)}, P_{b(0)}, T_b$$

Subject to:

Equality constraints:

$$\text{Process model: } f(z, x(z), x^-(z), u(z), v) = 0; [z_0, z_f]$$

Inequality constraints:

$$(1 \times 10^{-3} \text{ m}^3/\text{s}) \quad F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U \quad (2.43 \times 10^{-3} \text{ m}^3/\text{s})$$

$$(3.0 \text{ atm}) \quad P_{b(0)}^L \leq P_{b(0)} \leq P_{b(0)}^U \quad (41.0 \text{ atm})$$

$$(20 \text{ }^\circ\text{C}) \quad T_b^L \leq T_b \leq T_b^U \quad (44 \text{ }^\circ\text{C})$$

9.3.4.2 Optimisation Problem 2 (OP2)

- Given: inlet feed conditions, module specifications.
- Optimise: the inlet feed pressure, flow rate, and temperature.
- Minimise: the total specific energy consumption.
- Subject to: equality and inequality constraints of process model and linear bounds of optimisation variables, respectively.

Therefore, the mathematical expression of OP1 is as follows;

$$\text{Min} \quad E_4$$

$$F_{b(0)}, P_{b(0)}, T_b$$

Subject to:

Equality constraints:

$$\text{Process model: } f(z, x(z), x^-(z), u(z), v) = 0; [z_0, z_f]$$

Inequality constraints:

$$(1 \times 10^{-3} \text{ m}^3/\text{s}) \quad F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U \quad (2.43 \times 10^{-3} \text{ m}^3/\text{s})$$

$$(3.0 \text{ atm}) \quad P_{b(0)}^L \leq P_{b(0)} \leq P_{b(0)}^U \quad (41.0 \text{ atm})$$

$$(20 \text{ }^\circ\text{C}) \quad T_b^L \leq T_b \leq T_b^U \quad (44 \text{ }^\circ\text{C})$$

$$Rej_{NDMA} \geq 0.6273 \quad Rej_{NMEA} \geq 0.8864 \quad Rej_{NPYR} \geq 0.9454$$

The results of the RO process without an ERD (base case) of Fujioka et al. (2014) are reported in the first row of Table 9.3. The results of OP1 indicated the optimal values of NDMA, NMEA, and NPYR rejections as 0.80, 0.951, and 0.977, respectively. These show an increase of 27.5%, 7.3%, and 3.34% for the rejection of NDMA, NMEA, and NPYR, respectively, compared to those reported by Fujioka et al. (2014)

TABLE 9.3
Optimisation Results

No.	Optimisation problem	$F_{600} \times 10^3$, m ³ /s	T_{br} , °C	$P_{b(0)}$, atm	Rej (NDMA)	Rej (NMEA)	Rej (NPYR)	HPP 80% (Figure 9.1)	Energy Consumption kWh/m ³ HPP 80%+ERD 85% (Figure 9.2)	Boiler consumed power	Total energy consumption HPP 80%+ERD 85%+Boiler (Figure 9.2)	Comments
1	Base Case	2.43	20	10.100	0.6273	0.8864	0.9454	4.48	0	0	4.48	Fujioka et al. (2014) results
2	OP1	2.43 (opt)	20	35.41(opt)	0.80 (max)	0.951 (max)	0.977 (max)	3.678 (calc)	2.454 (calc)	0	2.454 (calc)	Optimised rejection at 20 °C
3		2.43 (opt)	42–44	35.41 (opt)	0.514	0.915	0.962	2.181 (min)	1.686 (min)	0.139	1.825	Calculated energy consumption at 44 °C
4	OP2	1.30 (opt)	20	12.98 (opt)	0.634 (calc)	0.8941 (calc)	0.949 (calc)	1.912 (min)	1.046 (min)	0	1.046	Optimised energy consumption at 20 °C
5		1.30 (opt)	42–44	12.98 (Selected)	0.514 (calc)	0.866 (calc)	0.936 (calc)	1.146 (min)	0.730 (min)	0.374	1.104	Calculated energy consumption at 44 °C

Inlet feed concentration of each N-nitrosamine is given in Table 9.1.
opt = optimised value; max = maximised value; min = minimised value
(Adapted from Al-Obaidi et al., 2018a)

(base case). The optimal feed flowrate of 2.43×10^{-3} m³/s, pressure 35.41 atm, and temperature at 20 °C were obtained corresponding to a considerable decrease in the total energy consumption from 4.48 kWh/m³ to 3.678 kWh/m³. A further reduction in energy consumption from 3.678 kWh/m³ to 2.454 kWh/m³ was observed with an ERD in place.

The total energy consumption decreased further as a result of increasing the temperature to 42 °C and 44 °C when compared to the base case of 20 °C. However, this increase of temperature had a significant impact on the rejections of NDMA, NMEA, and NPYR as 0.514, 0.915, and 0.962, respectively.

On the other hand, the optimisation results of OP2 show a significant reduction of the total energy consumption from 4.48 kWh/m³ to 1.912 kWh/m³ (operating at 20 °C) to 1.046 kWh/m³ (operating at 42–44 °C) for the RO configuration shown in Figure 9.1. A reduction of 57.3% in the specific energy consumption is noticed when compared to that of Fujioka et al. (2014). Although there is a noticeable improvement in the rejection of all pollutants at 20 °C, there is a noticeable decrease in the rejection of all pollutants at 40–42 °C compared to the base case of Fujioka et al. (2014). A further energy reduction is noticed when an ERD is used (configuration Figure 9.2). Additionally, the case total energy is increased when the boiler energy consumption is added to the calculations.

9.4 ADVANCED DESIGN OF A TWO-STAGE/TWO-PASS SPIRAL WOUND RO PROCESS FOR THE REMOVAL OF CHLOROPHENOL FROM WASTEWATER

Sundaramoorthy et al. (2011) reported a maximum rejection of 83% of chlorophenol from wastewater using an individual spiral wound RO process. Al-Obaidi et al. (2018b) have explored the efficiency of a two-stage/two-pass RO process for the removal of chlorophenol from wastewater considering model-based techniques. The model (Model X, Chapter 5) developed by Al-Obaidi et al. (2017b) was modified and used here.

9.4.1 TWO-STAGE/TWO-PASS RO PROCESS

The two-stage/two-pass RO process design is schematically presented in Figure 9.9. There are a total of seven pressure vessels—three in the first stage and two plus two in the second stage. A spiral wound commercial thin-film composite membrane type supplied by Ion Exchange (India) is used in each pressure vessel. The same membrane module was used by Sundaramoorthy et al. (2011) in their small-scale RO process. The membrane characteristics and the upper and lower bounds of the manufacturer's specifications are given in Table 9.4. The wastewater is fed to the three parallel pressure vessels of the first stage using a high-pressure pump. The retentates from these three pressure vessels are fed to two parallel pressure vessels (defined as stage 2). A booster pump was incorporated to raise the retentate pressure to the same value as the plant pressure one. The low-concentration permeate of the first stage plus the permeate collected from the second stage of the retentate processing are mixed and are fed to the two further parallel pressure vessels (referred to as stage 2)

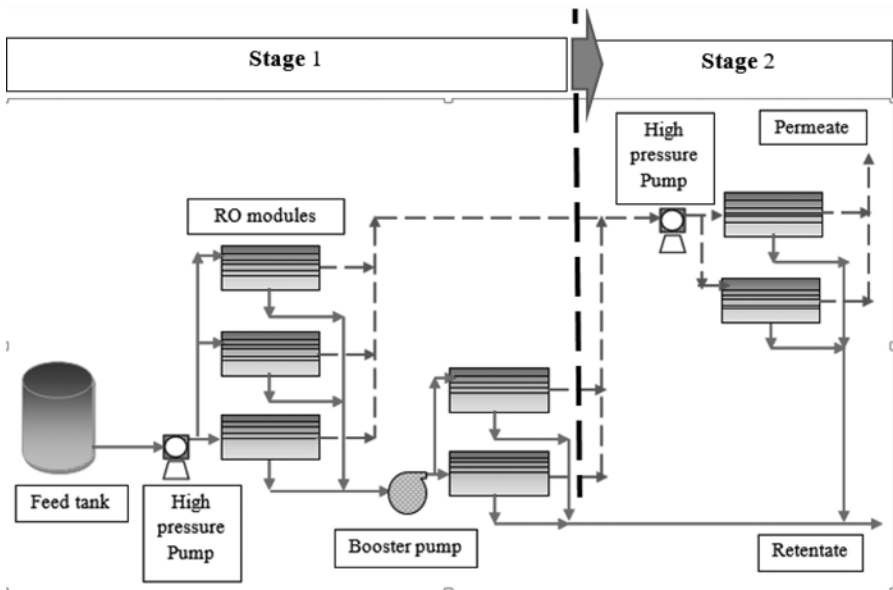


FIGURE 9.9 Schematic diagram of the proposed two-stage/two-pass RO process.

(Adapted from Al-Obaidi et al., 2018b)

TABLE 9.4

Membrane Characteristics and Lower and Upper Membrane Module Design Data

Parameter	Value	Parameter	Value
Supplier	Ion Exchange, India Ltd.	Effective membrane width (W)	8.4 (m)
Membrane brand and material	HM4040-LPE, Hydramem, TFC Polyamide	Effective membrane length (L)	0.934 (m)
Water transport parameter (A_w), measured at 30–32 °C	9.5188E-7 (m/atm s)	Maximum feed pressure (P_{fin})	24.77 (atm)
Chlorophenol transport parameter (B_s), measured at 30–32 °C	8.468E-8 (m/s)	Minimum flow rate	1E-3 (m ³ /s)
Reference temperature (T_0) (Sundaramoorthy et al., 2011)	31 (°C)	Maximum flow rate	1E-4 (m ³ /s)
Friction factor (b)	8529.45 (atm s/m ⁴)	Maximum pressure drop (atm)	1.38
Effective membrane area (A)	7.8456 (m ²)	Pump efficiency	0.85 (–)
Total membrane area of the plant	627.648 (m ²)	Booster pump efficiency	0.85 (–)
Height of the feed spacer (t_f)	0.0008 m	ERD efficiency	0.8 (–)
Feed cross section open area (A_s)	0.00672 (m ²)	Motor efficiency	0.98 (–)
Molecular weight of chlorophenol	128.6 (gm/mol)		

(Adapted from Al-Obaidi et al., 2018b)

for further polishing. This is why there was a need to also use a high-pressure pump to raise the pressure to be identical to that of the operating plant pressure. The maximum operating pressure considered is 20 atm. Finally, the retentate of the first and second stages are collected to form the main retentate disposed stream.

9.4.2 SENSITIVITY ANALYSIS

The influence of operating conditions on the process performance indicators was carried out via simulation to gain a deeper insight of the process before optimising it. Four different cases were considered with different operating pressure $P_{f(plant)}$, feed flow rate $Q_{f(plant)}$, and temperature $T_{(plant)}$, as shown below:

- 18 atm, 1.50E-3 m³/s, and 33 °C
- 15 atm, 7.749E-4 m³/s, and 32 °C
- 13 atm, 6.498E-4 m³/s, and 31 °C
- 12 atm, 5.40E-4 m³/s, and 30 °C.

The chlorophenol concentration $C_{f(plant)}$ of 6.226E-3 kmol/m³ was selected for all cases. Table 9.5 presents the simulation results of the four cases. The results clearly show an increase of chlorophenol rejection, which corresponds to a reduction in the permeate recovery and the energy consumption. However, the resulting chlorophenol rejection is noticeably higher than the one presented by Sundaramoorthy et al. (2011), clearly demonstrating the merits of the RO configuration considered.

9.4.3 OPTIMISATION OF THE TWO-STAGE/TWO-PASS SPIRAL WOUND RO PROCESS

Al-Obaidi et al. (2018b) maximised the chlorophenol rejection while optimising a number of operating and design parameters.

TABLE 9.5
Simulation Outputs of Two-Stage/Two-Pass RO Process for Chlorophenol Removal from Wastewater

Case	Total permeate concentration (kmol/m³)	Product flow rate (m³/s)	Total retentate concentration (kmol/m³)	Retentate flow rate (m³/s)	%Rejection (–)	%Recovery rate (–)	Energy consumption (kWh/m³)
1	2.154E-4	2.33E-4	7.329E-3	1.267E-3	96.54	15.51	5.71
2	3.389E-4	1.80E-4	8.005E-3	5.950E-4	94.56	23.20	3.35
3	4.508E-4	1.45E-4	7.890E-3	5.043E-4	92.76	22.38	2.97
4	5.865E-4	1.25E-4	7.922E-3	4.151E-4	90.58	23.13	2.66

Feed concentration = 6.226x10⁻³ kmol/m³

(Adapted from Al-Obaidi et al., 2018b)

The optimisation problem can be mathematically formulated as follows:

Max

$Q_{f(plant)}, P_{f(plant)}, T_{(plant)}$

$Rej_{(Total)}$

Subject to: Equality constraints:

Process model:

$f(x, u, v) = 0$

Inequality constraints of the plant: $5 \text{ atm } P_{f(plant)}^L \leq P_{f(plant)} \leq P_{f(plant)}^U \text{ 20 atm}$
 $3.0E-4 \text{ m}^3/\text{s } Q_{f(plant)}^L \leq Q_{f(plant)} \leq Q_{f(plant)}^U \text{ 3.0E-3 m}^3/\text{s}$
 $30 \text{ }^\circ\text{C } T_{(plant)}^L \leq T_{(plant)} \leq T_{(plant)}^U \text{ 33 }^\circ\text{C}$

Inequality constraints of the element:

$1.0E-4 \text{ m}^3/\text{s } Q_f^L \leq Q_f \leq Q_f^U \text{ 1.0E-3 m}^3/\text{s}$
 $5 \text{ atm } P_{f(in)}^L \leq P_{f(in)} \leq P_{f(in)}^U \text{ 20 atm}$
 $30 \text{ }^\circ\text{C } T^L \leq T \leq T^U \text{ 33 }^\circ\text{C}$
 $\Delta P_{drop} \leq 1.38$
 $Rec \geq 40\%$
 $1 \text{ kWh/m}^3 \leq E_{(Total)} \leq 2 \text{ kWh/m}^3$

Three cases are considered here. The optimisation results are presented in Table 9.6 (Case 1), in terms of maximum chlorophenol rejection, permeate recovery, and total energy consumption. However, the optimisation methodology has been extended to two other optimal solutions to further increase chlorophenol rejection with a penalty of increasing energy consumption within a permissible limit as highlighted in Table 9.6 and termed as Cases 2 and 3. Note, the pilot scale of an individual spiral wound RO process of Sundaramoorthy et al. (2011) resulted in 22% and 2.034 kWh/

TABLE 9.6
Optimisation Outputs of Two-Stage/Two-Pass RO Process for Chlorophenol Removal from Wastewater

Case	Operating conditions			Optimised parameters		
	Optimum flow rate, $Q_{f(plant)}$ m ³ /s	Optimum pressure, $P_{f(plant)}$ atm	Optimum temperature, $T_{b(plant)}$ °C	Max. rejection (%) $Rej_{(Total)}$ (–)	% Recovery, $Rec_{(Total)}$ (–)	Energy consumption, E_{Total} (kWh/m ³)
1	3.890E-4	13.24	33.0	93.33	40.00	1.95
2	5.176E-4	16.86	33.0	94.49	40.00	2.50
3	6.049E-4	19.30	33.0	95.02	40.00	2.87

Feed concentration = 6.226E-3 kmol/m³

(Adapted from Al-Obaidi et al., 2018b)

m³ of total water recovery and energy consumption, respectively. In this respect, the optimisation result of this study showed the possibility of attaining high chlorophenol rejection from 83% (obtained by Sundaramoorthy et al., 2011) to 93.3% as illustrated in Case 1 of Table 9.6. Also, the permeate recovery was increased by 81% (from 22% to 40%), with a decrease of 4% in the total energy consumption from 2.034 to 1.95 kWh/m³. Therefore, it is fair to mention that the optimisation has improved the process performance indicators compared to the one presented in the simulation results of Table 9.5. Specifically, Al-Obaidi et al. (2018b) have elaborated Cases 2 and 3 optimisation results with more focus on relaxing the total energy consumption between 2 and 3 kWh/m³. Table 9.6 presents a small improvement of chlorophenol rejection at the total energy consumption 2.50 kWh/m³ (Case 2) and 2.87 kWh/m³ (Case 3) when high pressures are applied. Case 1 therefore yields the most feasible option.

9.5 MULTI-STAGE AND MULTI-PASS RO NETWORKS FOR THE REMOVAL OF N-NITROSODIMETHYLAMINE-D6 FROM WASTEWATER

Al-Obaidi et al. (2018c) developed multi-stage and multi-pass of retentate and permeate reprocessing RO designs for the removal of N-nitrosodimethylamine-D6 (NDMA) from wastewater. The NDMA rejection, permeate recovery, and total energy consumption indicators were evaluated for each design via simulation using a comprehensive model, and the best design was determined. Optimisation of the best design was carried out in order to maximise the NDMA rejection with the lowest possible energy consumption while optimising a number of process parameters under feasible constraints.

9.5.1 MULTI-STAGE RETENTATE REPROCESSING DESIGN OF RO PROCESS

Al-Obaidi et al. (2018c) suggested different RO process networks based on a retentate reprocessing approach to remove NDMA from wastewater (Figure 9.10). Three network types of series, parallel, and tapered designs of six pressure vessels were used. Each pressure vessel contains three spiral wound membranes connected in series. The characteristics of the membrane modules and their associated technical specifications are given in Table 9.7.

All configurations in Figure 9.10 include a high-pressure pump with a maximum pressure of 40.463 atm and an efficiency of 80%.

9.5.1.1 Simulation of a Retentate Reprocessing Design of an RO Process

The simulation of the networks of a retentate reprocessing design of an RO process, as shown in Figure 9.10, is implemented using the operating conditions of 13 atm, 1000 ng/L, 8.9E-3 m³/s, and 25.3 °C of inlet pressure, concentration, flow rate, and temperature, respectively. In this respect, the NDMA rejection $Rej_{(plant)}$, total permeate recovery $Rec_{(plant)}$, and total energy consumption E are estimated. The simulation results are presented in Table 9.8. This indicates a poor rejection of NDMA between 38% and 40%.

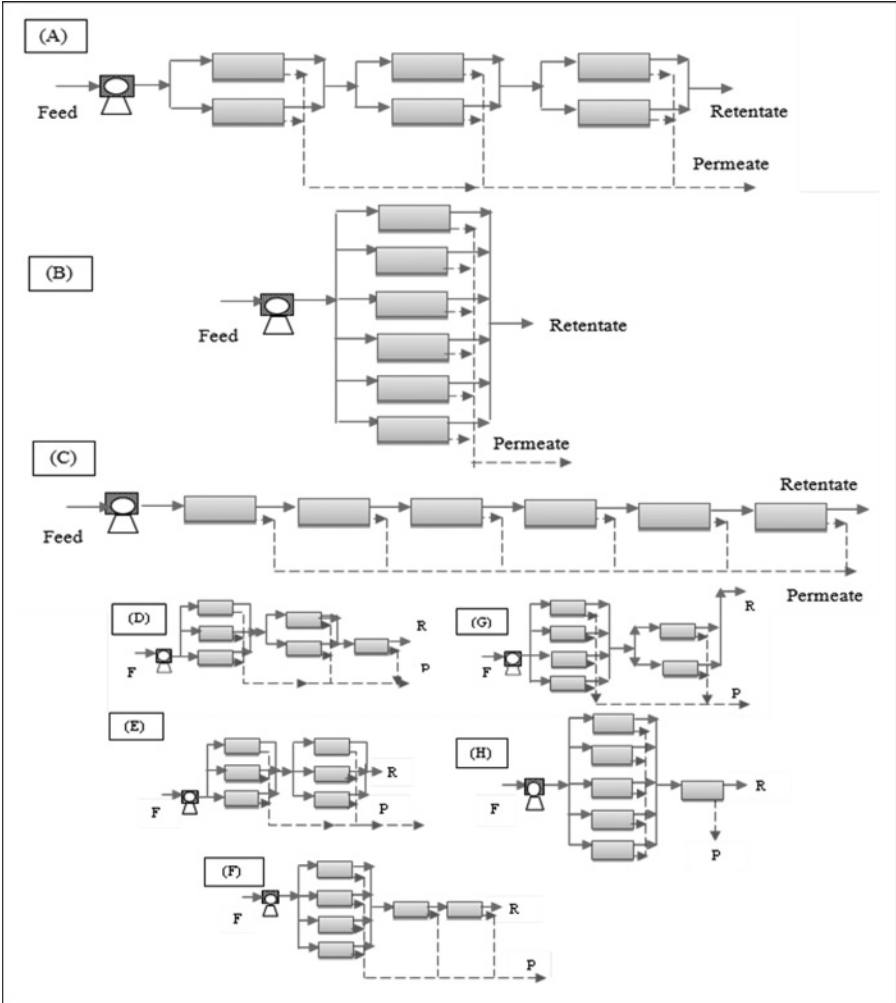


FIGURE 9.10 Retentate reprocessing design of multi-stage RO process for NDMA removal from wastewater (F: feed, P: permeate, R: retentate).

(Adapted from Al-Obaidi et al., 2018c)

Layout A has resulted in the maximum rejection. This might be attributed to the equal number of pressure vessels in each stage of layout A compared to other layouts. Also, the permeate recovery and total energy consumption range between 34% and 79% and 0.578 and 1.33 kWh/m³, respectively. The best permeate recovery and low energy consumption are noticed in layouts B, G, and H. This might be attributed to the maximum number of parallel pressure vessels in the first stage used in these layouts when compared to other layouts. A close look at the simulation results confirms that the permeate recovery has increased when the number of pressure vessels has increased, and this is despite the poor rejection of NDMA. Essentially, a reduced bulk velocity of each pressure vessel, due to the increased number of vessels

TABLE 9.7
Characteristics of the Spiral Wound Membrane Element

Make	Dow/FilmTec
Membrane type and configuration	BW30–400, Spiral wound, polyamide thin-film composite
Feed and permeate spacer thickness (m)	5.93E-4 and 5.50E-4
Hydraulic diameter of the feed spacer channel (m)	8.126E-4
Effective membrane area (m²)	37.2
Membrane length and width (m)	1 and 37.2
Water transport parameter (m/ atm s) at 28.8 °C	9.5096E-07
NDMA transport parameter (m/s) at 20 °C	5.35E-6*
NDMA molecular weight (kg/kmol)	74.05*
Spacer type	NALTEX-151–129
Spacer characteristics: A, n, ε (dimensionless)	7.38, 0.34, 0.9058

* Fujioka et al. (2014)
(Adapted from Abbas, 2005)

TABLE 9.8
Simulation of (A–H) Layouts of Retentate Reprocessing RO Process

Layout	Rej _(plant) (%)	Rec _(plant) (%)	E1 (kWh/m³)
A	40.43	72.90	0.627
B	38.69	79.16	0.578
C	40.53	34.37	1.331
D	39.71	76.548	0.597
E	39.15	77.29	0.591
F	39.44	76.97	0.594
G	38.85	78.28	0.584
H	38.74	78.69	0.581

(Adapted from Al-Obaidi et al., 2018c)

in the first stage, can lead to a higher permeate recovery. However, this reduces the mass transfer coefficient, which significantly influences the total rejection, due to an increase in the solute flux through the membrane.

The lowest permeate recovery and the worst energy consumption are achieved using layout C in comparison with other layouts. This also supports the previous argument where the pressure vessel of the first stage causes the highest feed flow rate causing the highest pressure drop and the lowest permeate permeation through the membrane. However, layout C yields the maximum NDMA rejection due to a reduction of the concentration polarisation. This was already confirmed by Fujioka et al. (2014) for NDMA removal and Farhat et al. (2013) for boron removal.

9.5.2 MULTI-STAGE PERMEATE REPROCESSING DESIGN OF AN RO PROCESS

The permeate reprocessing configuration of an RO process is used to improve the poor rejection of NDMA obtained using a retentate reprocessing configuration. Figure 9.11 shows the suggested networks of permeate reprocessing scheme (I–L). In these configurations, the permeates of the first stage are collected and fed to the next one and so on. All configurations consider the use of an energy recovery device (ERD) to absorb the energy from the high-pressure retentate stream and deliver it to the low-pressure permeate stream.

9.5.2.1 Simulation of a Permeate Reprocessing Design of an RO Process

The simulation results for these configurations are presented in Table 9.9. For all configurations, the NDMA rejections are found to be higher than those obtained by retentate reprocessing configurations despite a significant decrease in the permeate recovery. This can be ascribed to the disposal of the high-concentration retentate stream without further processing in the tapered layout I. However, layout J has significantly improved the recovery ratio and energy consumption by the setting of 4:2 design of pressure vessels. However, the NDMA rejection has been compromised compared with configuration I.

To sum up, the permeate reprocessing scheme can have a high NDMA rejection despite a low permeate recovery.

9.5.3 MULTI-STAGE MULTI-PASS COMBINED PERMEATE AND RETENTATE REPROCESSING OF AN RO PROCESS

Figure 9.12 presents a schematic diagram of the combined multi-stage permeate and retentate reprocessing design of RO process (layouts K, L, and M) as suggested by

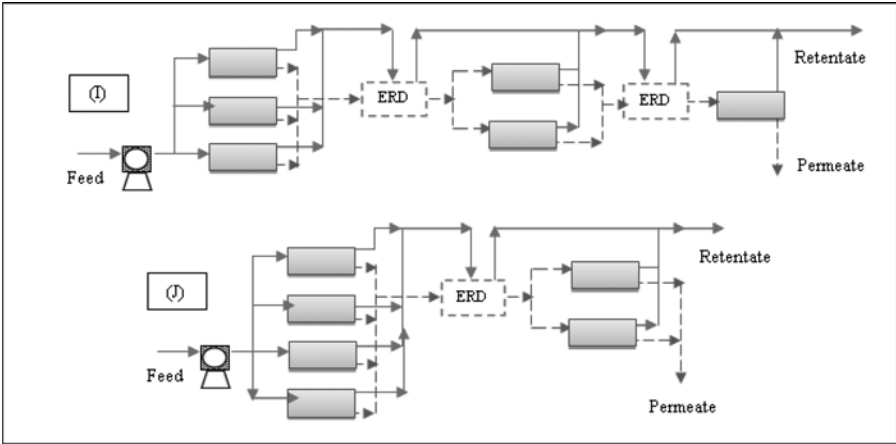


FIGURE 9.11 Permeate reprocessing design of multi-stage RO process for NDMA removal from wastewater.

(Adapted from Al-Obaidi et al., 2018c)

TABLE 9.9
Simulation of (I–J) Layouts of Permeate Reprocessing RO Process

Layout	$Rej_{(plant)} (-)$	$Rec_{(plant)} (-)$	E2 (kWh/m ³)
I	85.035	9.941	3.276
J	73.120	22.920	1.323

(Adapted from Al-Obaidi et al., 2018c)

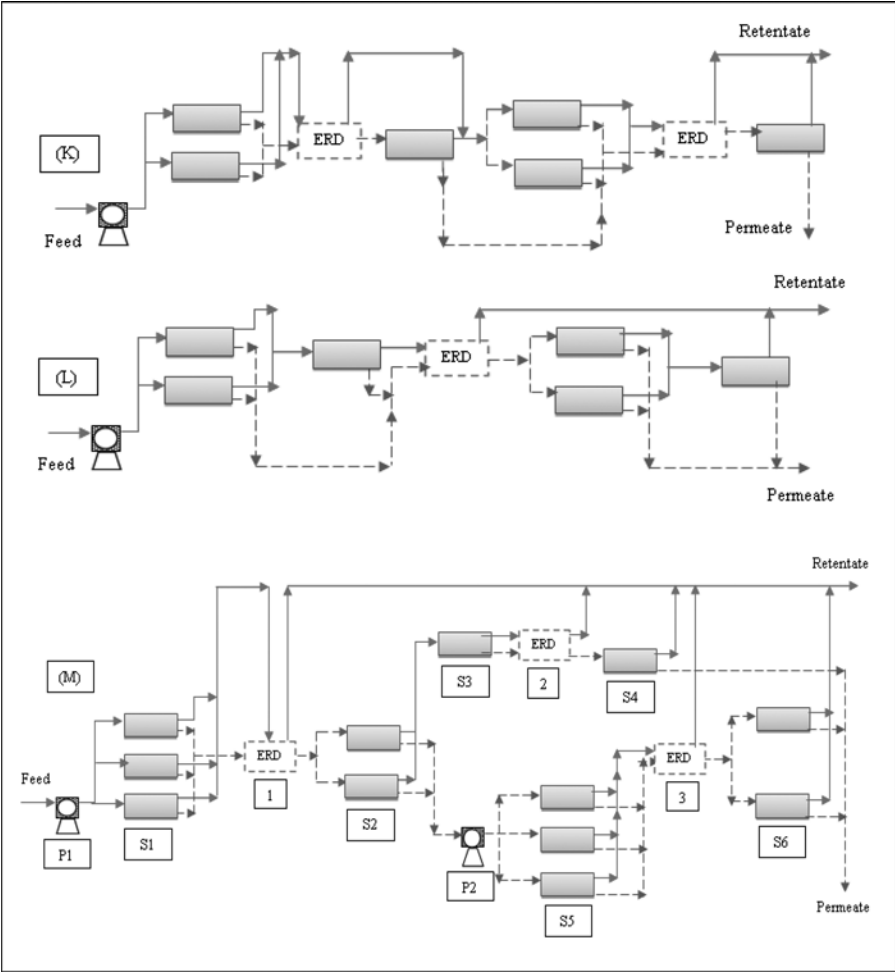


FIGURE 9.12 Permeate and retentate reprocessing design of multi-stage RO process for NDMA removal from wastewater.

(Adapted from Al-Obaidi et al., 2018c)

Al-Obaidi et al. (2018c). Configurations K to L use six pressure vessels as shown in Figures 9.10 and 9.11. However, configuration M has twelve pressure vessels, two high-pressure pumps, and three ERDs. This configuration includes three series membrane elements in each pressure vessel of stages S1, S2, S5, and S6, and one membrane element in each pressure vessel of stages S3 and S4.

9.5.3.1 Simulation of Advanced Design of RO Process

Between layouts K and L, layout K provides a higher NDMA removal but lower permeate recovery. However, layout L demands a lower energy consumption (Table 9.9). Moreover, layouts K and L entail a significant reduction of energy consumption compared to layouts I and J presented in Figure 9.11. However, the chlorophenol rejections of layouts K and L are less than layouts I and J, with achieving the best permeate recovery of 27.28%with layout L.

For configuration M, a noticeable elevation of NDMA rejection of 87.13% was achieved with 11.17% and 3.19 kWh/m³ of permeate recovery and energy consumption, respectively. The two high-pressure pumps were set at a similar operating pressure of 13 atm. Again, it seems that the issue of total permeate recovery has remained in the proposed layout M.

9.5.4 OPTIMISATION OF MULTI-STAGE MULTI-PASS PERMEATE-RETENTATE REPROCESSING RO PROCESS

The optimisation of configuration M (Figure 9.12) was considered by Al-Obaidi et al. (2018c) to maximise the removal of NDMA from wastewater with a permeate recovery of 40% (set as constraint). This was done by manipulating the operating variables such as total feed flow rate and pressure at fixed feed concentration of 1000 ng/L. The maximum pressure drop based on the membrane specifications was set at 0.987 atm. Table 9.11 shows the bounds of different parameters within which the optimisation is carried out. The energy consumption was constrained at 3 kWh/m³, to be roughly lower than the energy consumption of a large-scale seawater RO plant at roughly 3.5 kWh/m³ (Wei et al., 2017).

The optimisation problem was formulated as:

- Given: the feed conditions and membrane module specifications.
- Optimise: the feed pressure, flow rate, temperature, and feed pressure of stage 5 (S5).

TABLE 9.10
Simulation of (K–M) Layouts of Permeate Reprocessing RO Process

Layout	Rej _(plant) (%)	Rec _(plant) (%)	E2 (kWh/m ³)
K	76.1	8.62	1.17
L	68.1	27.28	0.77
M	87.1	11.17	3.19

(Adapted from Al-Obaidi et al., 2018c)

TABLE 9.11
Parameter Bounds

Parameter	Value	Parameter	Value
Max. operating temperature of Case 1	30	Max. pressure drop (atm)	0.987
Max. operating temperature of Case 2	45	Max. feed flow rate (m³/s)	5.363E-3
Max. operating pressure (atm)	40.46	Min. feed flow rate (m³/s)	1.008E-3

(Adapted from Abbas, 2005)

- Maximise: the NDMA removal.
- Subjected to: the equality and inequality constraints.

The mathematical representation of the optimisation problem as follows:

$$Max$$

$$Q_{f(plant)}, P_{f(in)(plant)}, P_{f(in)(S5)}, T_{(plant)}$$

$$Rej_{(NDMA)}$$

Subjected to:

Equality constraints:

Process model $f(x, u, v) = 0$

Inequality constraints:

$$Q_{f(plant)}, P_{f(plant)}, T_{(plant)}$$
$$P_{f(in)(plant)}^L \leq P_{f(in)(plant)} \leq P_{f(in)(plant)}^U$$
$$P_{f(in)(S5)}^L \leq P_{f(in)(S5)} \leq P_{f(in)(S5)}^U$$
$$T_{(plant)}^L \leq T_{(plant)} \leq T_{(plant)}^U$$

Inequality constraints of the element:

$$Q_f^L \leq Q_f \leq Q_f^U$$
$$P_{f(in)}^L \leq P_{f(in)} \leq P_{f(in)}^U$$
$$T^L \leq T \leq T^U$$
$$\Delta P_{drop} \leq 0.987$$
$$Rec(plant) \geq 40\%$$
$$E2 < 3.0$$

9.5.4.1 Optimisation Results

A range of 20 to 30 °C was chosen as the minimum and maximum temperatures of the first optimisation case to investigate the process performance.

Table 9.12 shows the optimisation results of layout M. For Case 1, NDMA rejection was 92.487% with a permeate recovery of 40% and an energy consumption of 2.664 kWh/m³. The rejection rate is very high compared to that obtained in all the retentate

TABLE 9.12
Optimisation Results of Advanced Layout M at Fixed Feed Concentration of 1000 Ng/L of NDMA

Case	The decision variables					The response variables		
	$Q_{f(plant)}$ (m ³ /s)	$P_{f(in) (plant)}$ (atm)	$T_{(plant)}$ (°C)	$P_{f(in)(stage5)}$ (atm)	$Rej_{(NDMA)}$ (%)	$C_P (NDMA)$ (ng/L)	$Rec_{(plant)}$ (%)	E2 (kWh/ m ³)
1	7.9526E-3	23.50	30.0	40.46	92.49	75.13	40.00	2.664
2 A	8.4510E-3	22.20	36.0	38.11	92.38	76.25	40.00	2.500
B	9.8887E-3	23.39	41.6	40.03	93.11	68.9	40.00	2.612

(Adapted from Al-Obaidi et al., 2018c)

and permeate reprocessing schemes presented in earlier sections. The high NDMA removal leads to a permeate concentration of 75 ng/L, which is lower than the recommended concentration of 100 ng/L by the World Health Organization (WHO, 2008).

The Case 2 optimisation has been formulated to further minimise the total energy consumption of layout M. Therefore, the optimisation formulation of Case 1 (described in section 9.5.4) has been considered for Case 2 optimisation except that the maximum energy consumption is set lower than that obtained in Case 1 (2.664 kWh/m³). Therefore, a new energy consumption constraint has been added to the optimisation formulation which is $E2 < 2.664 \text{ kWh/m}^3$.

To achieve this target of lower energy consumption of layout M, the optimisation limits of operating temperature have been set to 20 °C and a maximum allowed temperature of 45 °C, compared to the limits of Case 1 at 20 to 30 °C. In other words, the impact of feed temperature will be investigated in Case 2.

Table 9.12 shows that Case 2A has maintained the high removal of NDMA of 92.38% as well as yielded a lower energy consumption compared to Case 1. This is due to the enhanced water permeation constant due to the increasing temperature. Specifically, Case 2 presented two options (A and B) of operating conditions, which can be used to maintain a fixed permeate recovery of 40% as mainly constrained in the optimisation problem. Option B (with a different feed flow rate), on the other hand, provides a lower permeate concentration with a penalty of a slightly higher energy consumption when compared to option A.

To sum up, layout M can provide a high removal of NDMA at an acceptable permeate recovery and a competitive energy consumption. The optimisation results, especially the NDMA removal, have been found to be close to the results of Fujioka et al. (2018), but with a very high recovery ratio compared to those.

9.6 PERMEATE AND RETENTATE STREAM RECYCLING OF MULTI-STAGE RO PROCESS FOR CHLOROPHENOL REMOVAL FROM WASTEWATER

In the literature can be found several attempts to study the influence of permeate and retentate stream recycling options on the RO process performance. For instance,

Al-Bastaki and Abbas (2003) applied the permeate recycling scheme and confirmed an optimum value of 25% of permeate recycling at a fixed feed flow rate seawater desalination RO process, which mitigated freshwater concentration by around 15%. However, a penalty of reduced water recovery by around 22% was associated with this product improvement. Sarkar et al. (2008) applied partial retentate recycle on a small-scale brackish water RO desalination process and concluded that a fixed product flow rate can be maintained by increasing the operating temperature, which corresponds to an increased retentate recycling ratio.

Al-Obaidi et al. (2019a) evaluated the impact of different scenarios of recycling the permeate, retentate, and permeate-retentate streams on the performance of a multi-stage RO wastewater treatment system for the removal of chlorophenol from wastewater. The multi-stage RO simulation was performed using the calibrated version of the model developed by Al-Obaidi et al. (2017b) (Model X, Chapter 5). This included the calculation of the total recovery rate, permeate product concentration, overall chlorophenol rejection, and energy consumption, which were all associated with the performance of the system. Also, the effects of temperature, pressure, feed flow rate, and concentration on the whole performance of constant and variable plant feed flow rate cases of permeate recycle design were analysed to gain deeper insight of the process.

9.6.1 DESCRIPTION OF MULTI-STAGE PERMEATE AND RETENTATE STREAMS RECYCLING OF AN RO PROCESS

Al-Obaidi et al. (2019a) developed several three-stage configurations with four pressure vessels of permeate, retentate, and permeate and retentate recycling schemes as shown in Figure 9.13. All the configurations were designed as 2:1:1, where each pressure vessel contains one spiral wound membrane element. The specifications of this membrane are given in Table 9.4. A high-pressure pump of maximum 20 atm was used to drive the wastewater inside the pressure vessels at a fixed operating temperature of 31 °C.

A product stream of low-concentration chlorophenol was formed due to linking the permeates of all the stages while the retentate of high concentration was discharged. To carry out the recycling of permeate or retentate portions into the feed stream, splitters (flow-control valves) were used to regulate the requested portion and assess its influence on the process performance indicators. This also facilitated the comparison between a no-recycle scheme and a recycle one.

9.6.2 SIMULATION RESULTS

A simulation analysis of the proposed design, presented in Figure 9.13, was carried out in line with the membrane manufacturer of similar operating conditions of $6.226\text{E-}3$ kmol/m³, 15 atm, $5.166\text{E-}4$ m³/s, and 31 °C of feed concentration, pressure, flow rate, and temperature. The simulation consisted of two cases of fixed and variable feed flow rate of partial recycling of permeate and retentate streams, which were used to assess their influence on the process performance.

9.6.2.1 Case Study 1

A fixed fresh feed flow rate of $5.166\text{E-}4$ m³/s has been considered to assess its influence on process performance. The flow rate of the first stage will therefore increase

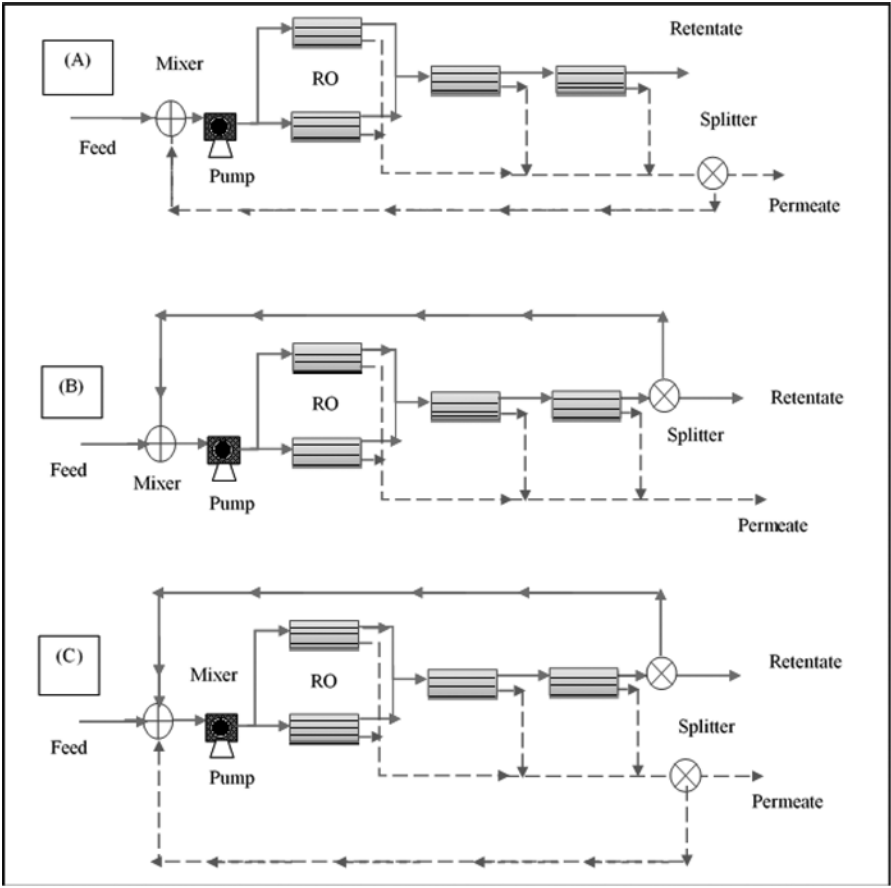


FIGURE 9.13 The proposed permeate, retentate, and permeate-retentate recycling design of multi-stage RO process.

(Adapted from Al-Obaidi et al., 2019a)

with the additional flow of the recycled stream. Figures 9.14 and 9.15 illustrate the influence of different ratios of permeate, retentate, and permeate and retentate streams on the permeate chlorophenol concentration, water recovery, and energy consumption, respectively. It is also noteworthy to mention that an equal ratio of permeate and retentate streams were used in the third configuration (C) of the permeate and retentate scheme.

Several conclusions can be drawn from Figures 9.14 and 9.15, and they include:

- Configuration A of Figure 9.13 gave the best design leading to a noticeable decrease in the chlorophenol permeate concentration. The reduction of inlet feed concentration is progressed due to the recycling of the low-concentration permeate compared to other configurations tested.

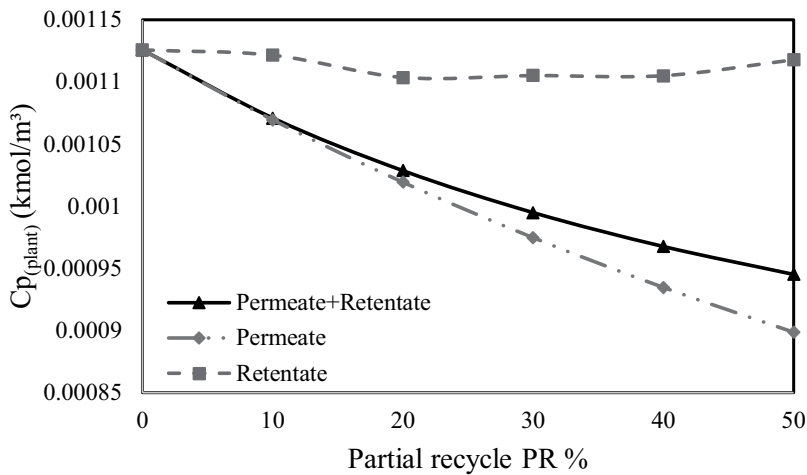


FIGURE 9.14 Influence of partial recycle ratio of permeate, retentate, and permeate + retentate streams on permeate concentration of Case 1.

(Adapted from Al-Obaidi et al., 2019a)

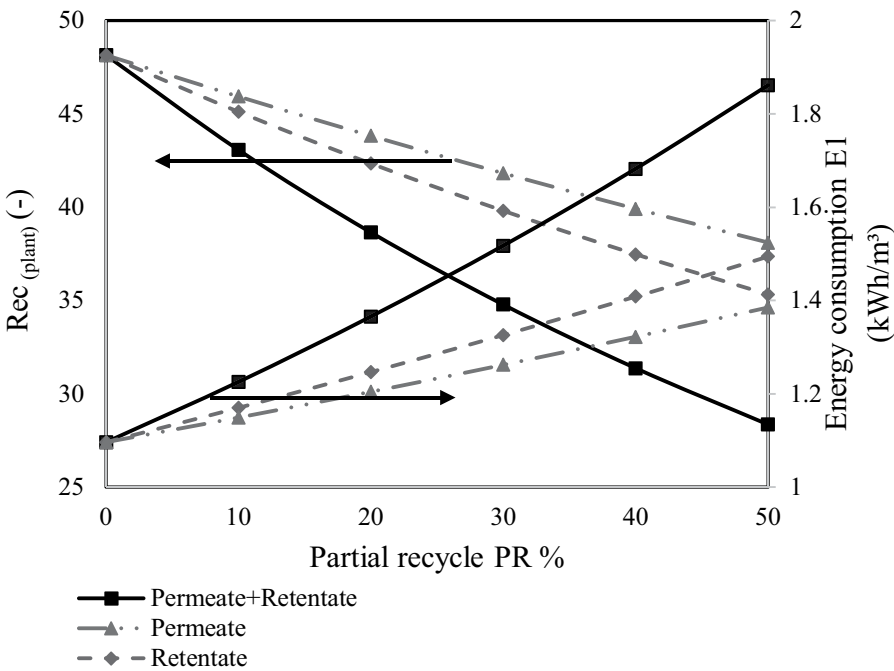


FIGURE 9.15 Influence of partial recycle ratio of permeate, retentate, and permeate + retentate streams on permeate recovery and energy consumption of Case 1.

(Adapted from Al-Obaidi et al., 2019a)

- The fixed fresh feed flow rate has demonstrated a reduction in the permeate recovery with an increase in the total energy consumption for all the configurations tested of A, B, and C as confirmed in Figure 9.18. The increase of bulk velocity in each compartment increased the pressure drop along the membrane length leading to a reduction in the permeated water through the membrane.
- Again, the permeate recycling scheme has shown the best permeate recovery and the lowest energy consumption compared to the other configurations of B and C.

9.6.2.2 Case Study 2

A fixed feed flow rate of $5.166\text{E-}4\text{ m}^3/\text{s}$ in the first stage is considered here. The fresh feed flow rate is reduced as a result of increasing the ratio of recycled stream. The simulation of Case 2 has been carried out using a fixed pressure and temperature. Figures 9.16 and 9.17 show the influence of recycled ratio of permeate and retentate streams on the chlorophenol permeate concentration, total permeate recovery, and energy consumption, respectively. A progressive decrease of permeate recovery for recycling the retentate stream was noticed compared to the case when recycling the permeate stream. The retentate recycling scheme was associated with the increased feed concentration of the first stage leading to a concentration polarisation and a reduction of water permeation, total permeate recovery, and increased energy consumption. On the other hand, recycling the permeate stream reduced the feed concentration of the first stage and the total permeate concentration, which had a positive impact on the permeate recovery and energy consumption.

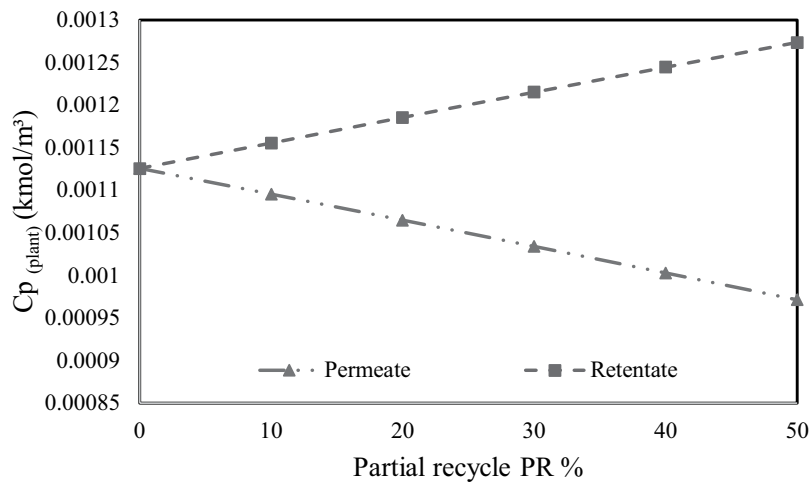


FIGURE 9.16 Influence of partial recycle ratio of permeate and retentate streams on chlorophenol permeate concentration of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

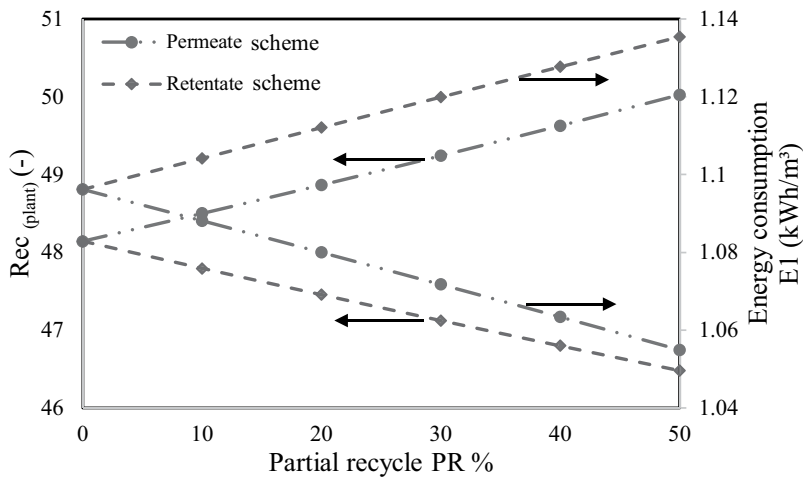


FIGURE 9.17 Influence of partial recycle ratio of permeate and retentate streams on permeate recovery and energy consumption of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

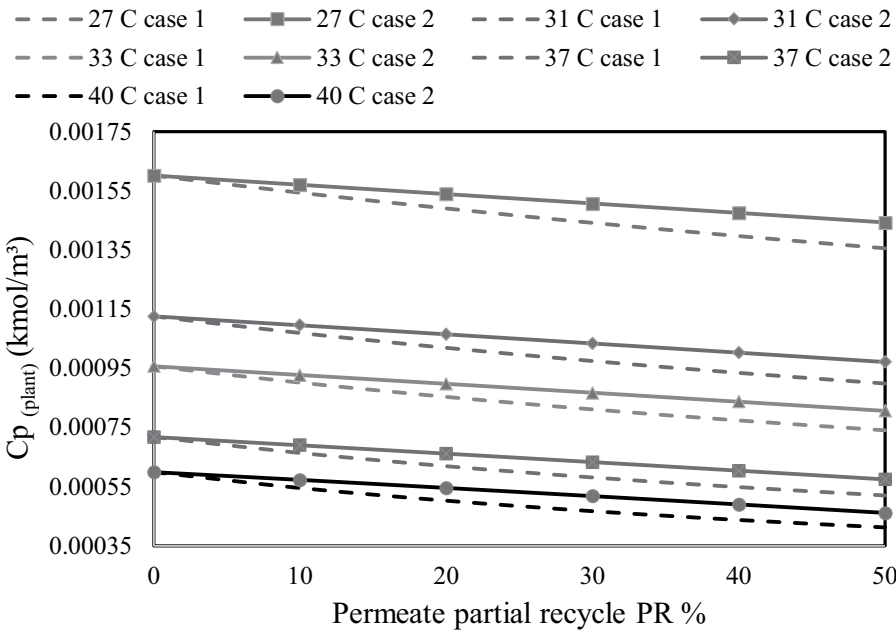


FIGURE 9.18 Influence of feed temperature on chlorophenol permeate concentration of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

To sum up, the simulation results of Cases 1 and 2 confirmed the merits of the recycling of the permeate stream and its consistency to mitigate the chlorophenol permeate concentration and the total energy consumption.

9.6.3 SENSITIVITY ANALYSIS OF OPERATING CONDITIONS

The influence of changing the feed temperature between 27 °C and 40 °C for the chlorophenol rejection and the total permeate recovery of permeate reprocessing design of an RO process based on Cases 1 and 2 of fixed and variable feed flow rate, respectively, was studied using a changing recycled permeate ratio between 0% and 50%. Increasing the temperature causes a reduction of the permeate concentration, a growth in the permeate recovery, and a chlorophenol rejection for Cases 1 and 2 as given in Figures 9.18 to 9.21.

Table 9.13 depicts the permeate chlorophenol concentration, permeate recovery, energy consumption, and chlorophenol rejection with and without the permeate recycle of Cases 1 and 2.

For Case 1, a significant decrease in the permeate recovery and the permeate concentration with a significant increase in the energy consumption at 27 and 40 °C respectively were noticed with 50% permeate recycle ratio when compared to zero permeate recycle (Table 9.13). However, an insignificant increase in the chlorophenol rejection was noticed in Case 1. For Case 2, the reduction in the permeate concentration and rejection and the improvement in the recovery ratio were noticed for both temperatures but with a decrease in rejection. Overall, Case 2, with the high-temperature operation, was better in terms of recovery ratio and rejection with an acceptable permeate concentration and energy consumption.

Figure 9.18 confirms a higher decrease of chlorophenol concentration in Case 1 compared to Case 2, where any increase of temperature would support the

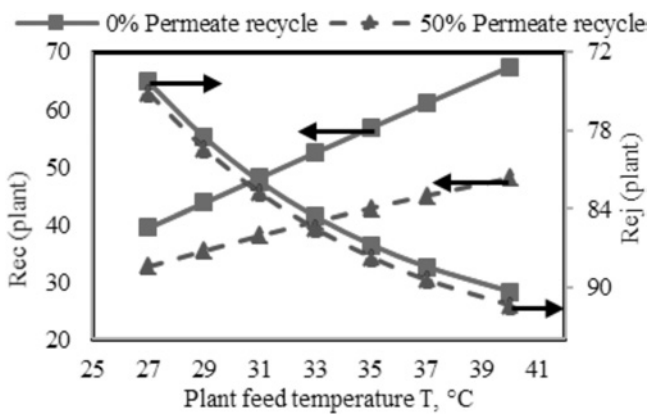


FIGURE 9.19 Influence of feed temperature on permeate recovery and chlorophenol rejection of permeate recycle design of Case 1.

(Adapted from Al-Obaidi et al., 2019a)

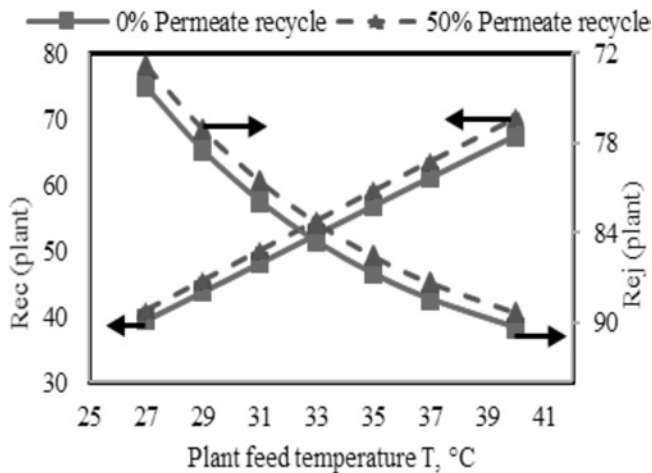


FIGURE 9.20 Influence of feed temperature on permeate recovery and chlorophenol rejection of permeate recycle design of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

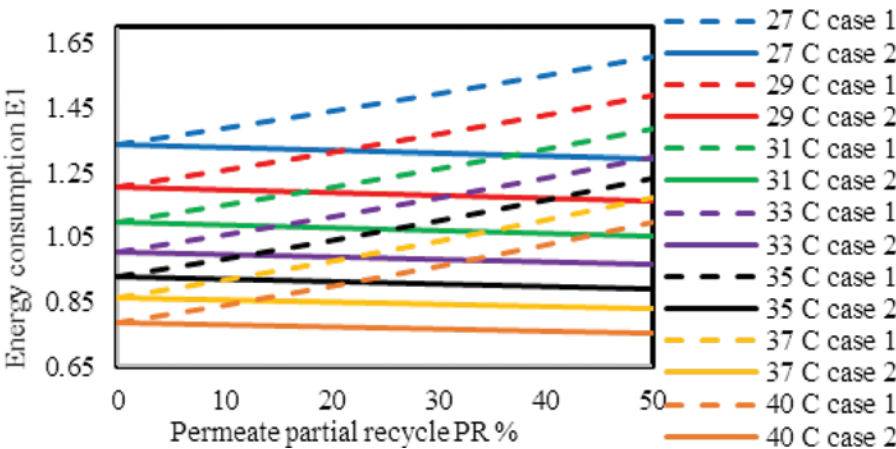


FIGURE 9.21 Influence of feed temperature on total energy consumption of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

concentration decrease. For all the temperature ranges used and all recycle ratios, Case 1 required a higher consumption of energy when compared to Case 2, as presented in Figure 9.21.

The impact of the feed pressure ranged between 13 and 20 atm on the process performance indicators of permeate recycling scheme at a recycling ratio between 0% and 50% in Cases 1 and 2, as more particularly shown in Figures 9.22 to 9.25.

TABLE 9.13
Simulation Results: Base Case = No Recycle; Case 1 = Variable Feed to Stage 1 (Fixed Fresh Feed); Case 2 = Fixed Feed to Stage 1 (Variable Fresh Feed)

Operating parameters	Case	Permeate recycle ratio %	Parameter variation	Cp _(plant) × 10 ³ kmol/m ³	Operating conditions and improvement calculations							
					Improvement (+, −) %	Rec _(plant) %	Improvement (+, −) %	E1 (kWh/m ³)	Improvement (+, −) %	Rej _(plant) %	Improvement (+, −) %	
Temp. (27–40 °C)	Base	0	27	1.60	–	39.5	–	1.33	–	74.3	–	
		1	50	27	1.36	+15.3	32.7	–17.13	1.61	–21.05	75.2	+1.22
		2	50	27	1.44	+9.89	40.9	+3.49	1.29	+3.00	72.8	–1.93
	Base	0	40	0.59	–	67.4	–	0.78	–	90.4	–	
		1	50	40	0.41	+31.18	48.1	–28.71	1.09	–39.74	91.4	+1.15
		2	50	40	0.46	+22.98	70.3	+4.32	0.75	+3.84	89.3	–1.14
Pressure (13–20 atm)	Base	0	13	1.13	–	39.2	–	1.16	–	81.8	–	
		1	50	13	0.95	+15.93	31.7	–19.19	1.44	–23.75	82.3	+0.65
		2	50	13	1.00	+11.64	40.5	+3.29	1.13	+3.18	80.9	–1.15
	Base	0	20	1.19	–	68.1	–	1.03	–	80.8	–	
		1	50	20	0.83	+30.01	52.6	–22.79	1.33	–29.53	83.1	+2.83
		2	50	20	0.99	+17.15	71.7	+5.13	0.98	+4.88	78.0	–3.40
Feed Conc. (6.226E–3–9.5E–3 kmol/m ³)	Base	0	6.226E–3	1.12	–	48.1	–	1.09	–	81.9	–	
		1	50	6.226E–3	0.89	+20.17	38.1	–20.85	1.38	–26.34	82.8	+1.12
		2	50	6.226E–3	0.97	+13.71	50.0	+3.90	1.05	+3.76	80.6	–1.65
	Base	0	9.5E–3	1.51	–	44.1	–	1.19	–	84.1	–	
		1	50	9.5E–3	1.22	+18.75	35.9	–18.32	1.46	–22.43	84.8	+0.79
		2	50	9.5E–3	1.30	+13.46	46.1	+4.67	1.14	+4.46	83.1	–1.17

(Adapted from Al-Obaidi et al., 2019a)

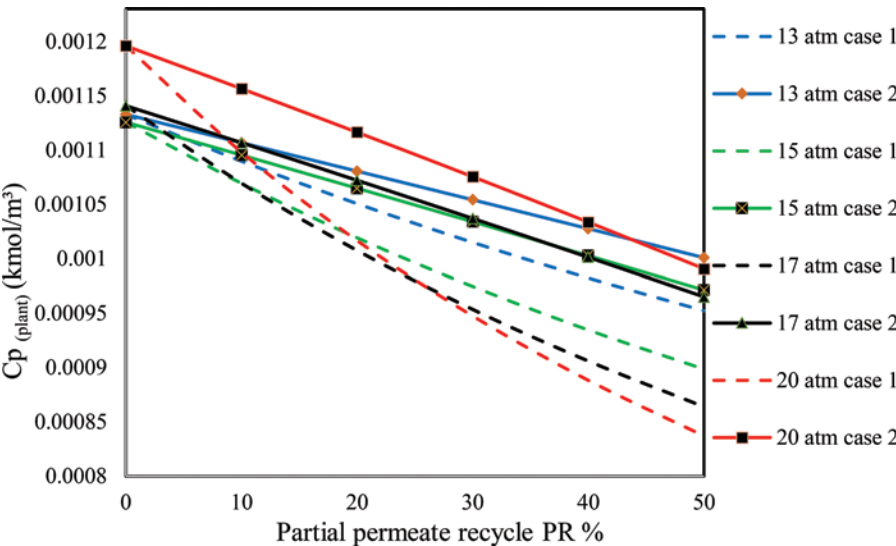


FIGURE 9.22 Influence of feed pressure on chlorophenol permeate concentration of permeate recycle design of Cases 1 and 2.
(Adapted from Al-Obaidi et al., 2019a)

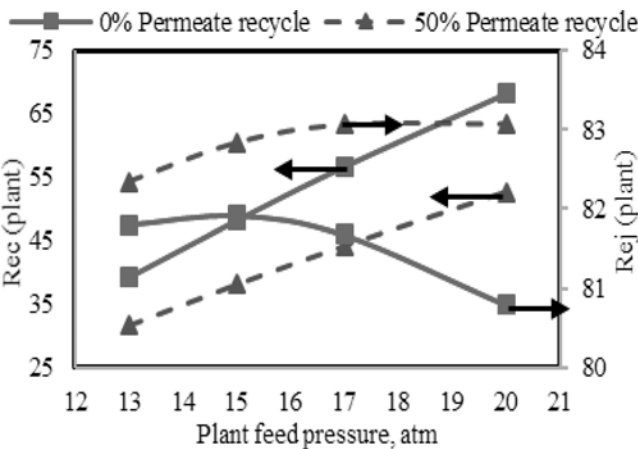


FIGURE 9.23 Influence of feed pressure on permeate recovery and chlorophenol rejection of permeate recycle design of Case 1.
(Adapted from Al-Obaidi et al., 2019a)

Although the actual values varied, the impact of pressure on the trend (increase/reduction) of all performance parameters were the same as those obtained by changing the operating temperature (Table 9.13).
Figures 9.23 and 9.24 present an optimum value of feed pressure corresponding to the maximum chlorophenol removal from wastewater.

Again, Case 2 with a high-pressure operation was better in terms of the recovery ratio with an acceptable permeate concentration, rejection, and energy consumption. However, Case 1 with a high-pressure operation was better in terms of permeate concentration and rejection but with an extremely poor recovery ratio and higher energy consumption (Table 9.13 and Figure 9.25).

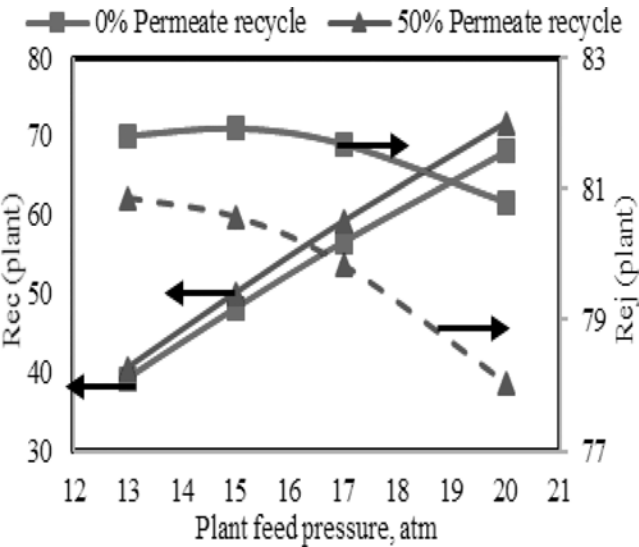


FIGURE 9.24 Influence of feed pressure on permeate recovery and chlorophenol rejection of permeate recycle design of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

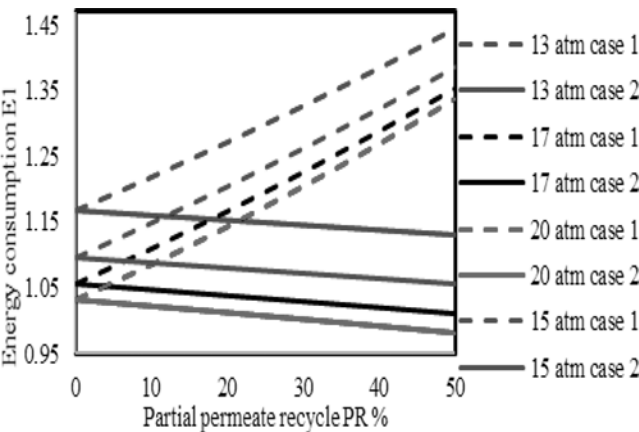


FIGURE 9.25 Influence of feed pressure on total energy consumption of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

The impact of changing the fresh feed concentration from 6.226E-3 to 9.5E-3 kmol/m³ on the permeate recovery and chlorophenol removal of the RO permeate recycling process of Cases 1 and 2 for the recycling ratio between 0% and 50% is shown in Figures 9.26 and 9.27, respectively. Increasing the feed concentration led to a reduction of permeate recovery but with an increase of the chlorophenol rejection

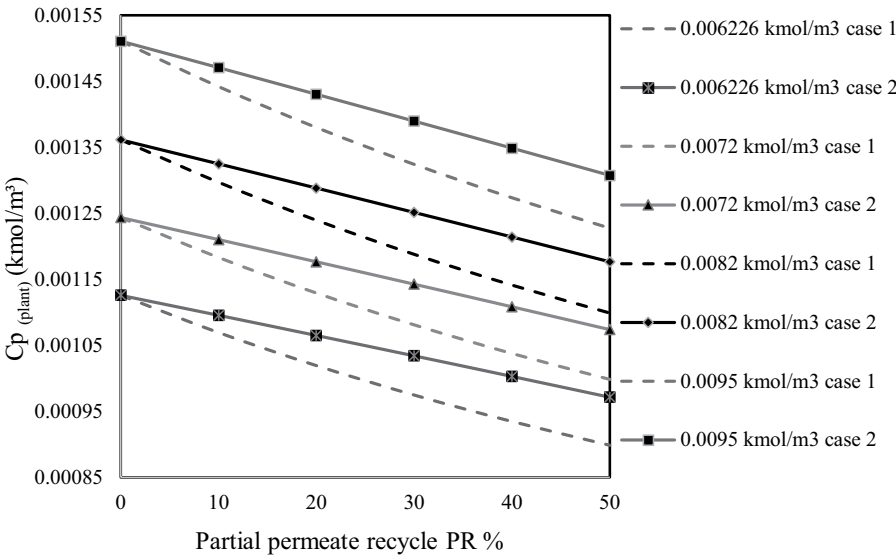


FIGURE 9.26 Influence of feed concentration on chlorophenol permeate concentration of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

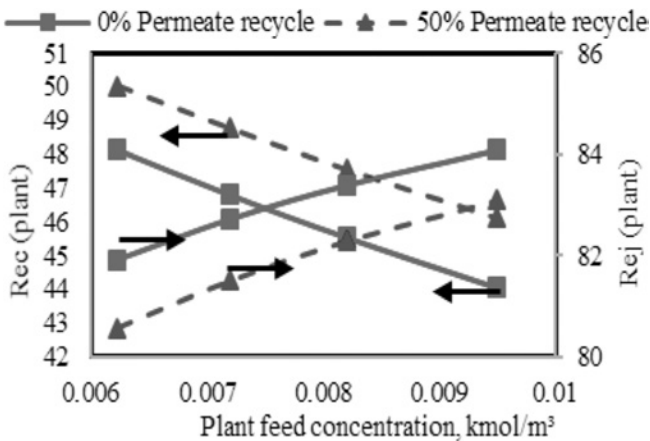


FIGURE 9.27 Influence of feed concentration on permeate recovery and chlorophenol rejection of permeate recycle design of Case 1.

(Adapted from Al-Obaidi et al., 2019a)

(Figure 9.27) for all cases. Again, although the actual values varied, the impact of the fresh feed concentration on the trend (increase/reduction) of all performance parameters were the same as those obtained by changing the operating temperature or pressure (Table 9.13).

Overall, Case 2 with a low feed concentration operation was better in terms of the recovery ratio and the energy consumption with an acceptable permeate

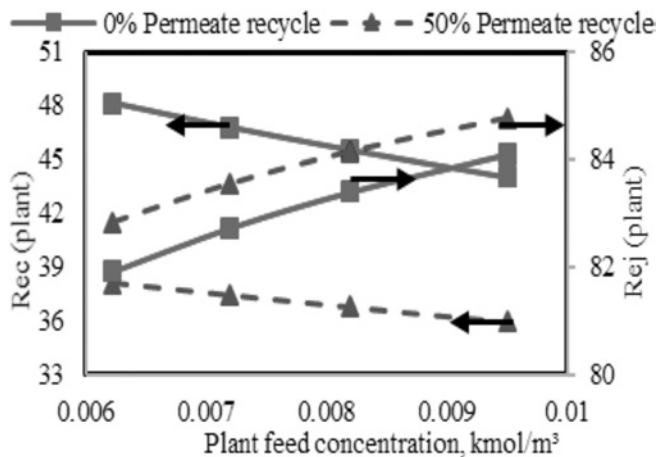


FIGURE 9.28 Influence of feed concentration on permeate recovery and chlorophenol rejection of permeate recycle design of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

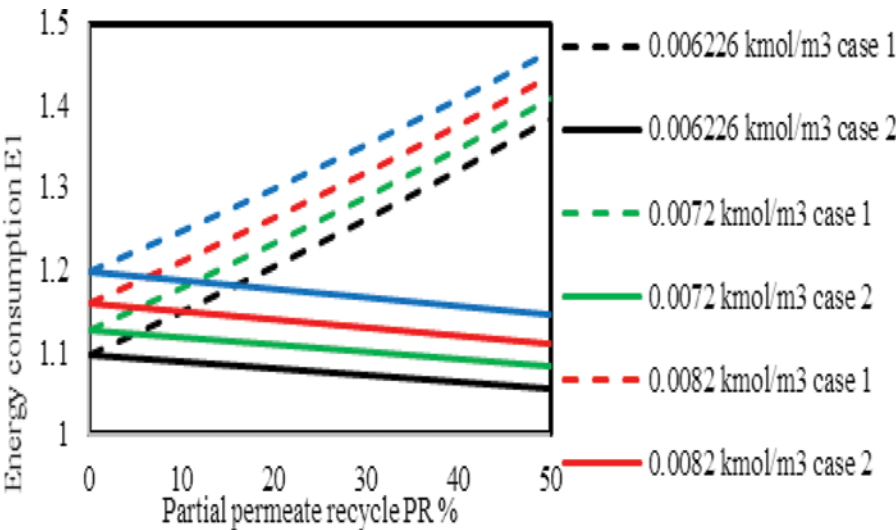


FIGURE 9.29 Influence of feed concentration on total energy consumption of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

concentration and rejection. However, in terms of rejection, Case 1 with a higher fresh feed concentration operation was better but with a poor recovery ratio and a higher energy consumption (Table 9.13).

Undoubtedly, increasing the concentration would increase the osmotic pressure that retards the water flux and permeate permeation. This also is responsible for the growth of the concentration polarisation and solute permeation through the membrane pores. This would then increase the permeate concentration at the permeate channel as demonstrated in Figure 9.26.

On the other hand, the chlorophenol removal increased for Cases 1 and 2, as more particularly shown in Figures 9.27 and 9.28, respectively. This has occurred despite the increase of the chlorophenol permeate concentration due to an incomparable simultaneous increase of both bulk and permeate concentrations that controlled the whole rejection. Finally, Figure 9.29 expresses a reduction of energy consumption as a result of applying Case 2 to Case 1 for all the considered percentages of partial permeate recycle.

9.6.4 IMPACT OF THE FRESH FEED FLOW RATE ON THE PERFORMANCE OF A PERMEATE RECYCLING RO PROCESS

The impact of two different fresh feed flow rates of 3.5E-4 and 7E-4 m³/s at fixed feed concentration pressure and temperature are considered here to evaluate the performance of the process.

The variation of chlorophenol permeate concentration as a result of increasing the fresh feed flow rate from 3.5E-4 to 7E-4 m³/s for the permeate recycle ratio between 0% and 50% of Cases 1 and 2 is presented in Figure 9.30. This easily shows

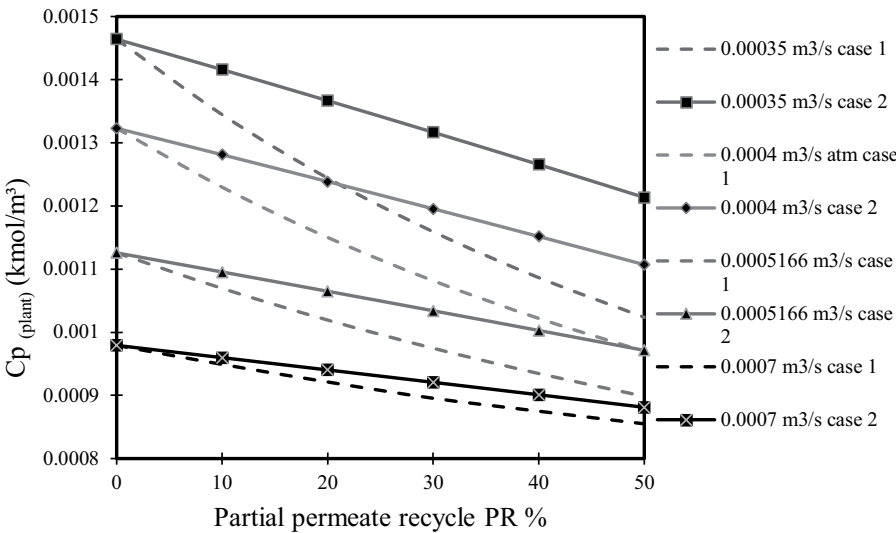


FIGURE 9.30 Influence of feed flow rate on chlorophenol permeate concentration of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

a continuous reduction of permeate chlorophenol concentration as a result of increasing the fresh feed flow rate, where Case 1 showed a higher reduction in concentration than did Case 2.

The influence of fresh feed flow rate on the permeate recovery and chlorophenol removal is illustrated in Figures 9.31 and 9.32 against the variation of the permeate recycle ratio between 0% and 50% for Cases 1 and 2, respectively. The figures showed a reduction of permeate recovery and an increase in the chlorophenol rejection when compared to the influence of feed pressure and temperature. Figures 9.31 and 9.32 show that increasing the feed flow rate from $3.5\text{E-}4$ to $7\text{E-}4$ m^3/s has caused an improvement in the chlorophenol rejection of 10.18% (from 5.87% to 13.93%) in no-recycle mode and 50% permeate recycle in Cases 1 and 2, respectively. On the other hand, a reduction of 53%, 51.4%, and 54.6% in the no-recycle mode and 50% ratio of permeate recycle in Cases 1 and 2, respectively, were recorded for total recovery rate. Increasing the feed flow rate causes a reduction of concentration polarisation, which improves the rejection parameter. However, this reduces the water permeation and the total permeate recovery. This would therefore explain the increase of energy consumption due to the reduction of permeate collected, as demonstrated in Figure 9.33. Table 9.14 presents the advantages and disadvantages of applying a 50% ratio of permeate recycle in both Cases 1 and 2, compared to a no-recycle mode. The simulation results at $3.5\text{E-}4$ and $7\text{E-}4$ m^3/s without a recycle were used as the base values to assess the improvement (+, -) of Cases 1 and 2. Table 9.14 shows a decrease of the permeate chlorophenol concentration of 30% and 12.66% of 50% of the permeate recycle ratio for Case 1 at $3.5\text{E-}4$ and $7\text{E-}4$ m^3/s , respectively, compared to the base case of a no-recycle mode. On the other hand, a reduction of permeate chlorophenol concentration of 17% and 10% at $3.5\text{E-}4$ and

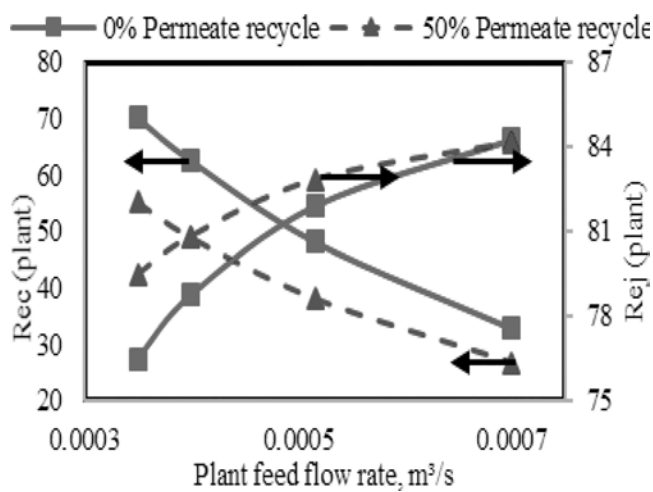


FIGURE 9.31 Influence of feed flow rate on permeate recovery and chlorophenol rejection of permeate recycle design of Case 1.

(Adapted from Al-Obaidi et al., 2019a)

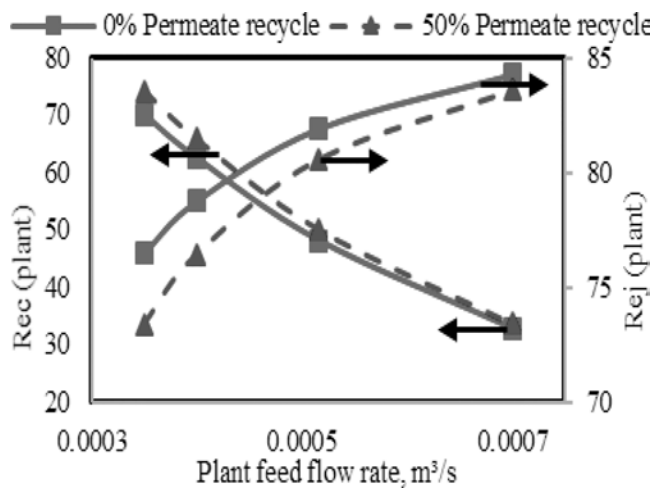


FIGURE 9.32 Influence of feed flow rate on permeate recovery and chlorophenol rejection of permeate recycle design of Case 2.

(Adapted from Al-Obaidi et al., 2019a)

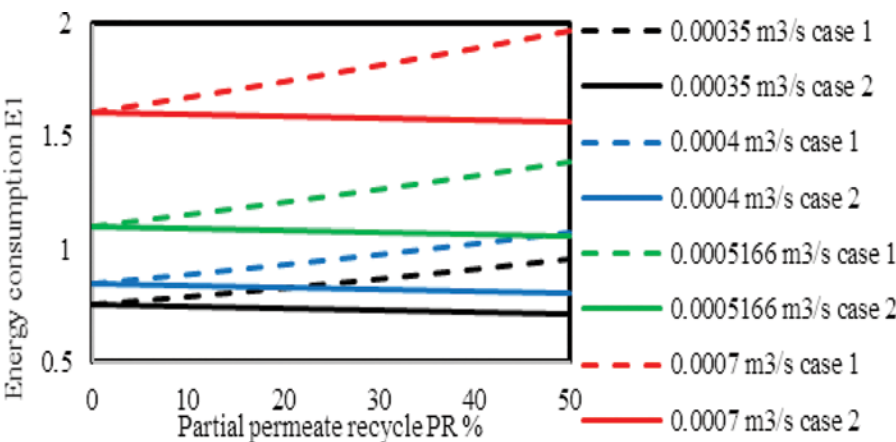


FIGURE 9.33 Influence of feed flow rate on total energy consumption of permeate recycle design of Cases 1 and 2.

(Adapted from Al-Obaidi et al., 2019a)

7E-4 m³/s, respectively, were noticed for 50% the permeate recycle ratio of Case 2, compared to the no-recycle mode. Table 9.14 confirms that the low feed flow rate at 50% permeate recycle ratio for Case 1 strengthens the permeate concentration of chlorophenol compared to Case 2 in the no-recycle mode. Interestingly, increasing the feed flow rate to 7E-4 m³/s would significantly improve the permeate concentration of chlorophenol.

TABLE 9.14
Simulation Results of External Feed Flow Rate of Case 3 Based on Cases 1 and 2 of 0% and 50% Permeate Recycle Mode

TABLE 9.14 Simulation Results of External Feed Flow Rate of Case 3 Based on Cases 1 and 2 of 0% and 50% Permeate Recycle Mode													
Case	Permeate recycle ratio %	Feed Flow Rate (m ³ /s)	Cp _(plant) × 10 ³ (kmol/m ³)	Operating conditions and improvement calculations							Rej _(plant) %	Improvement (+, −) %	Improvement (+, −) %
				Improvement (+, −) %	Rec _(plant) (%)	Improvement (+, −) %	E1 (kWh/m ³)	Improvement (+, −) %					
Base	0	3.5E-4	1.46	−	70.18	−	0.75	−	76.48	−	−	−	
	50	3.5E-4	1.02	+30.07	55.17	−21.37	0.95	−27.19	79.48	+3.91	+3.91		
	50	3.5E-4	1.21	+17.11	74.23	+5.76	0.71	+5.45	73.35	−4.08	−4.08		
Base	0	7E-4	0.97	−	32.84	−	1.60	−	84.27	−	−	−	
	50	7E-4	0.85	+12.66	26.79	−18.41	1.96	−22.57	84.41	+0.16	+0.16		
	50	7E-4	0.88	+10.01	33.67	+2.51	1.56	+2.45	83.57	−0.82	−0.82		
(Adapted from Al-Obaiddi et al., 2019b)													

(Adapted from Al-Obaidi et al., 2019b)

9.7 DESIGN OF A MULTI-STAGE RO PROCESS FOR THE REMOVAL OF CHLOROPHENOL FROM WASTEWATER

RO membrane systems are often used as a network of a number of stages, which include several pressure vessels of membrane modules. The design of a multi-stage RO process should meet the requirements of the separation process, including environmental and economic perspectives. The following sections outline a new design of multi-stage RO process used to remove chlorophenol from wastewater.

9.7.1 DESCRIPTION OF THE MULTI-STAGE RO PROCESS

Figure 9.34 shows the schematic diagram of Al-Obaidi et al. (2019b) of a three-stage RO wastewater treatment configuration connected in series. The whole system consists of eight blocks where each block contains ten parallel pressure vessels. Moreover, each pressure vessel contains only one membrane module. Specifically, stages 1 and 3 have three parallel blocks compared to stage 2 of two blocks. The design of stage 2 is designed in such a way to satisfy the limits of operation, thus securing the lower feed flow rate due to the incorporation of the permeate streams of stage 1, compared to other stages. A membrane type (Ion Exchange, India Ltd., 7.846 m²) was used by Sundaramoorthy et al. (2011) for the removal of chlorophenol from wastewater in a spiral wound module and is considered in this simulation. The total membrane area in the three-stage RO process is 627.65 m². Membrane

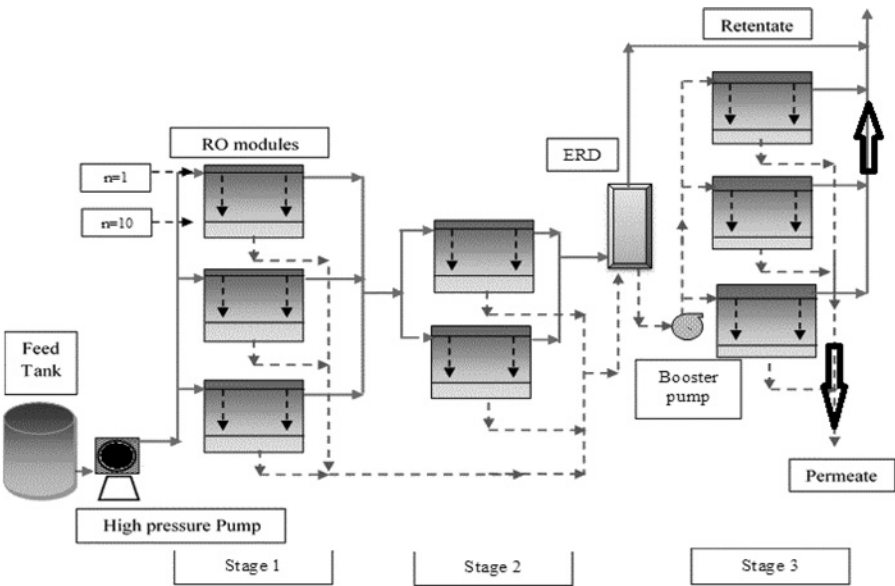


FIGURE 9.34 Schematic diagram of the proposed RO process (80 membrane elements, 1 membrane for each pressure vessel, and 10 membranes in each block).

(Adapted from Al-Obaidi et al., 2019b)

specifications, including the transport parameters of water and chlorophenol and the friction parameter, are given in Table 9.4 based on Sundaramoorthy et al. (2011). The configuration shown in Figure 9.34 includes an ERD and a booster pump, where the permeate from stages 1 and 2 are blended and pressurised before being fed to stage 3 for further processing. This accelerates the transfer of energy from the high-pressure retentate to the low-pressure feed of stage 3. Both stages 1 and 3 can therefore be said to be working at the same operating pressure, where the booster pump raises the operating pressure of stage 3 to its desired value.

To get a better insight of the process performance in terms of chlorophenol rejection, total recovery rate, and energy consumption in a multi-stage RO process, a detailed simulation of the process is carried out using a modified version of the model (Model X, Chapter 5) developed by Al-Obaidi et al. (2017b). Model X was calibrated to be consistent with the RO configuration of the current study. Moreover, a specific equation to calculate the energy consumption was included due to the existence of booster pump and energy recovery device besides the high-pressure pump.

9.7.2 SENSITIVITY ANALYSIS OF OPERATING CONDITIONS

The sensitivity analysis was carried out by measuring the impact of the variation of one operating parameter at a time, while other parameters are fixed, on the performance of the multi-stage RO process in terms of chlorophenol rejection, total recovery rate, and specific energy consumption.

Figure 9.35 depicts the simulation results of the total recovery rate and chlorophenol rejection at various feed pressures and fixed feed flow rate, concentration, and

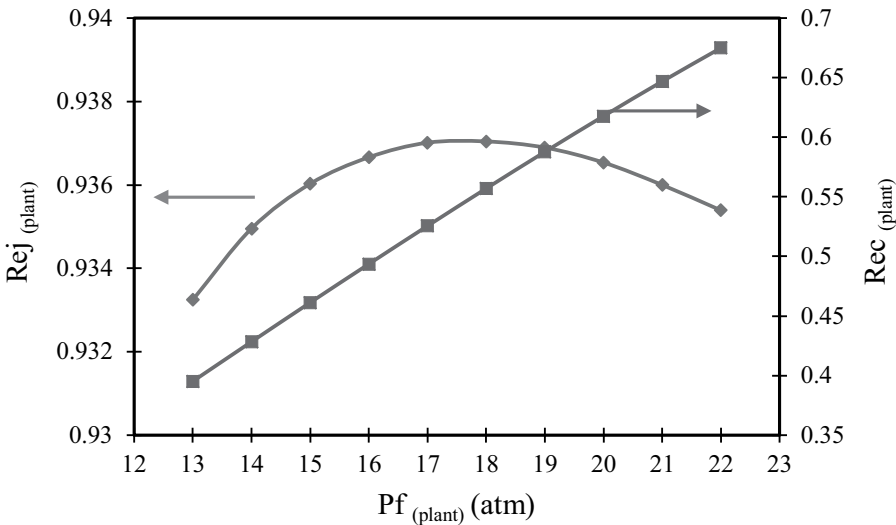


FIGURE 9.35 The plant rejection and recovery rate versus the operating pressure.

(Adapted from Al-Obaidi et al., 2019b)

temperature of 0.006 m³/s, 6.226E-3 kmol/m³, and 33 °C, respectively. Increasing the pressure by about 70% results in a significant increase of the water recovery. However, the rejection remains relatively constant up to 17 atm (between 93.3% and 93.7%) and then decreases above 17 atm. This is due to build-up of solute concentration on the membrane surface, which causes a higher osmotic pressure. This slightly decreases the rejection up to a given pressure. The insignificant impact of the operating pressure on rejection can be attributed to several factors, as will be discussed in the following sections.

The variation of chlorophenol rejection $Rej_{(stage)}$ and chlorophenol flux $Js_{(stage)}$, water recovery $Rec_{(stage)}$, and permeate concentration $Cp_{(stage)}$ of stages 1, 2, and 3 are illustrated in Figures 9.36 and 9.37, respectively.

The chlorophenol rejection in stages 1 and 2 is insignificantly changed as a result of increasing the pressure, as shown in Figure 9.36. This is due to a significant increase in solute flux, especially in stage 2. This holds a higher solute flux compared to stage 1 due to a higher feed concentration. In this respect, stage 3 receives the permeates of stages 1 and 2 and uses the same operating plant pressure and therefore works at a lower feed concentration. This leads to an increase in the water recovery compared to stages 1 and 2, as shown in Figure 9.37. These conditions help reduce the solute flux in stage 3 (Figure 9.36) as well as the permeate concentration (Figure 9.37). However, a positive relationship between the operating concentration and the solute rejection was noticed where the solute rejection increases when the concentration increases. This may be attributed to an increase in the membrane solute isolation intensity (Al-Obaidi and Mujtaba, 2016). Stage 3 yields therefore the

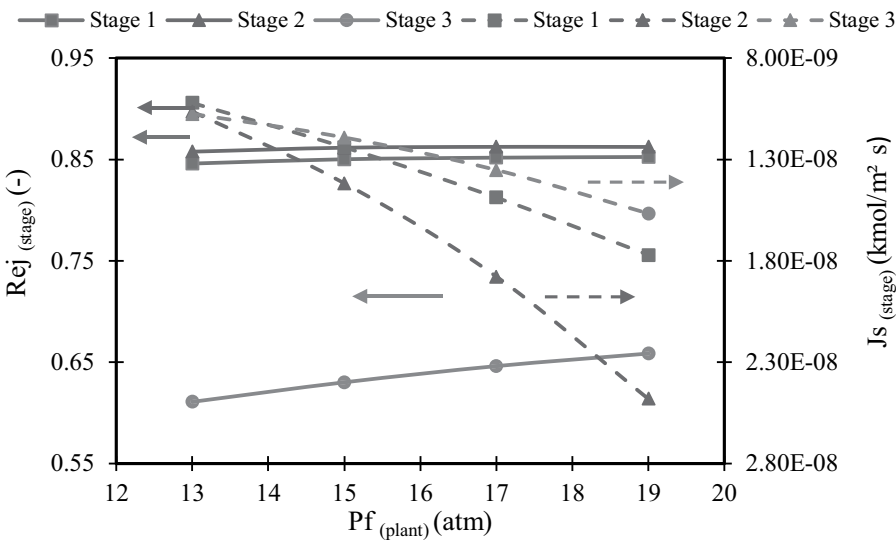


FIGURE 9.36 The effect of pressure on chlorophenol rejection and solute flux for three stages.

(Adapted from Al-Obaidi et al., 2019b)

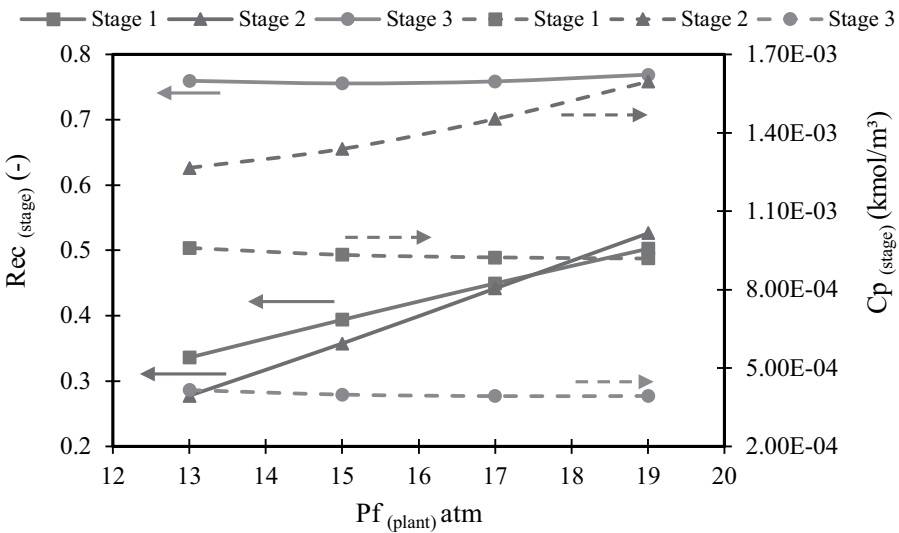


FIGURE 9.37 The effect of pressure on recovery rate and permeate concentration for three stages.

(Adapted from Al-Obaidi et al., 2019b)

lowest chlorophenol rejection with a relatively constant total chlorophenol rejection against the feed pressure (Figure 9.35).

Figure 9.37 confirms a significant increase in the water recovery of stages 1 and 2 with the pressure due to the increased water flux. However, stage 3 yields the highest recovery compared to other stages despite its low rate of increase. This is due to the low feed concentration of stage 3, which aids the water flux.

Figure 9.38 shows the impact of operating pressure on the total specific energy consumption SEC and the total product flow rate $Qp_{(plant)}$ at fixed operating conditions. A significant growth of the total product flow rate at the expense of higher energy consumption (to maintain higher pressures) is noticed. However, the use of an ERD has helped reduce the net total energy consumption.

Secondly, the impact of the feed flow rate variation at a fixed operating pressure, concentration, and temperature of 15 atm, 6.226E-3 kmol/m³, and 33 °C, respectively, versus chlorophenol rejection and water recovery is illustrated in Figure 9.39.

It can be seen that a variation of the feed flow rate from 0.0045 m³/s to 0.014 m³/s at fixed other operating parameters increases the chlorophenol rejection by around 2.5% (Figure 9.39). However, the consequence of the feed flow rate variation causes a significant reduction in the total water recovery at around 65.4%. Clearly, the solute flux through the membrane decreases with a slight improvement in the water flux as a result of increasing the bulk velocity. This improves the rejection parameter due to a reduction in the concentration polarisation (Farhat et al., 2013).

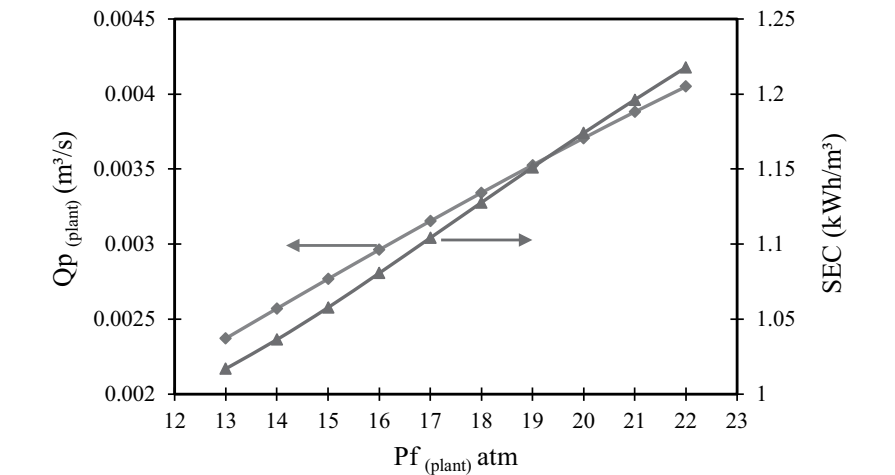


FIGURE 9.38 The effect of pressure on the product flow rate and specific energy consumption.
(Adapted from Al-Obaidi et al., 2019b)

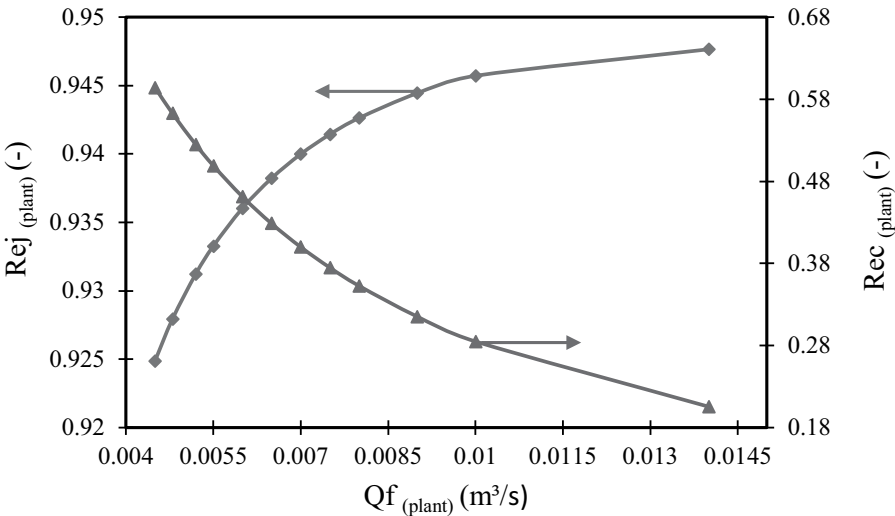


FIGURE 9.39 The effect of feed flow rate on the plant rejection and recovery rate.
(Adapted from Al-Obaidi et al., 2019b)

The reduction in the concentration polarisation has improved the water flux, which is equivalent to a 7.6% increase in the total permeate flow rate $Qp_{(plant)}$, as shown in Figure 9.40. However, the total plant recovery rate kept on falling because of the feed flow rate variation, as shown in Figure 9.39. This is mainly due to the

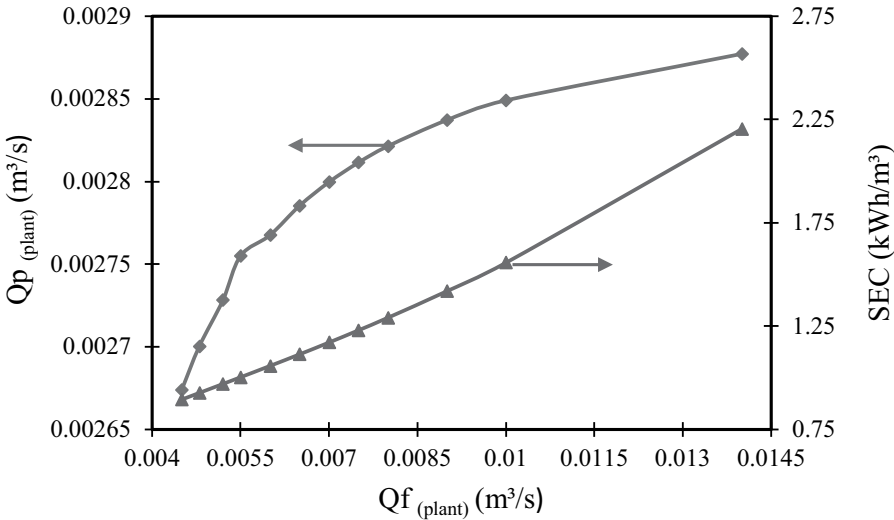


FIGURE 9.40 The effect of feed flow rate on the product flow rate and specific energy consumption.

(Adapted from Al-Obaidi et al., 2019b)

dependence of the total permeate flow rate on the product of the last stage of the process, as shown in Figure 9.34.

Figure 9.40 shows an increase in the specific energy consumption SEC of around 146.4% due to the variation of feed flow rate corresponding to an enhancement of the permeate flow rate of around 7.6%.

Figure 9.41 shows the effect of the feed concentration variation from 0.000778 kmol/m³ to 0.012 kmol/m³ (equivalent to 100 ppm to 1543 ppm) on the chlorophenol rejection and water recovery at fixed feed pressure, flow rate, and temperature of 15 atm, 0.006 m³/s, and 33 °C, respectively.

Increasing the feed concentration has a positive impact on the chlorophenol rejection, where it progressively rises at low feed concentrations and then slowly increases at high feed concentrations. Al-Obaidi and Mujtaba (2016) confirmed the possibility of increasing the chlorophenol rejection as a result of increasing the feed concentration, which is caused by the rise of the membrane intensity when removing the chlorophenol. However, working at a high feed concentration medium actually increases the osmotic pressure and retards the progress of rejection. On the other hand, increasing the feed concentration has a negative impact on water recovery due to the deterioration of water flux because of the rising osmotic pressure. Increasing the feed concentration causes 20% increase of chlorophenol rejection and 16.2% decrease of water recovery.

Increasing the feed concentration causes a reduction in the total permeate flow rate $Q_{p(plant)}$ as given in Figure 9.42, with a minimum value of the specific energy consumption SEC between 0.003891 and 0.006226 kmol/m³ of the feed concentration.

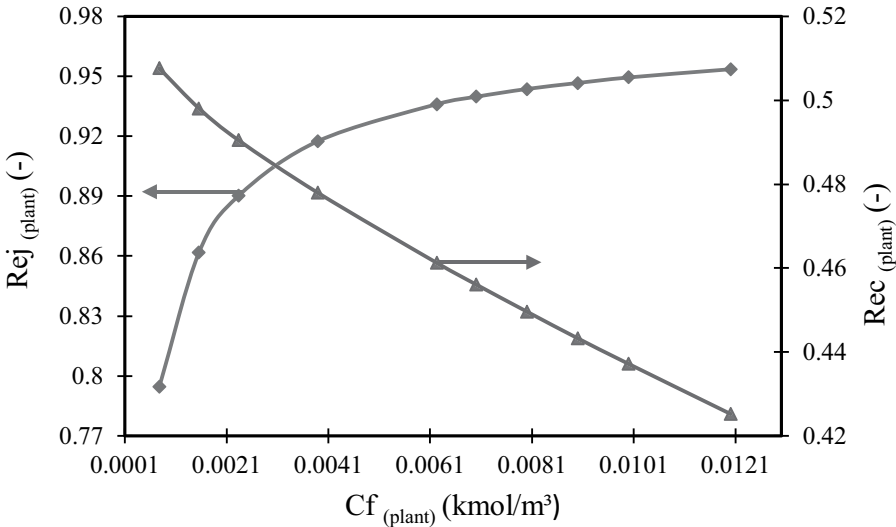


FIGURE 9.41 The effect of feed concentration on the plant rejection and recovery rate.
(Adapted from Al-Obaidi et al., 2019b)

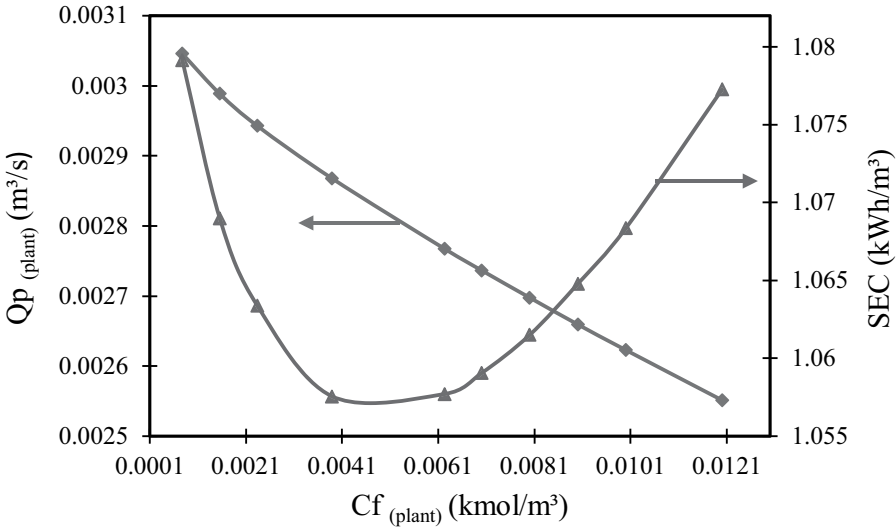


FIGURE 9.42 The effect of feed concentration on the product flow rate and specific energy consumption.
(Adapted from Al-Obaidi et al., 2019b)

The *SEC* includes the power consumption of the high-pressure pump and the booster pump, minus the energy saved in the ERD.

Increasing the feed concentration causes an improvement of the total retentate feed flow rate of stage 2 and a reduction of the retentate pressure of stage 2. This is followed by a continuous reduction in the total permeate flow rate at stages 1 and 2. This means a continuous reduction of the total inlet flow rate of the booster pump, which essentially decreases the overall power consumption. Additionally, the energy recovery of ERD is in fact increased due to the rise in the feed concentration and retentate flow rate of stage 2. In contrast, increasing the feed concentration causes an increase of the power consumption of the high-pressure pump, which reduces the total permeate flow rate $QP_{(plant)}$. Figure 9.43 depicts an illustration of the effect of the feed concentration on the power consumptions of the high-pressure pump and the booster pump, which is recovered by ERD. This clearly shows the advantages of using an ERD to save energy.

Finally, the impact of temperature variation from 30 to 40 °C (33% increase) at a fixed feed pressure, concentration, and flow rate of 15 atm, 6.226E-3 kmol/m³, and 0.006 m³/s, respectively, on the chlorophenol rejection and the total water recovery are shown in Figure 9.44. It is worth noting that the temperature is varied within the regulated limits of the membrane manufacturer and in line with the conditions of industrial effluents. The temperature increase has a positive impact on both the chlorophenol rejection (9.7%) and water recovery (37.7%) (Figure 9.44). This observation is in line with the findings of several other researchers such as Madaeni and Koocheki (2006), Kim et al. (2009), and Ntavou et al. (2016). Essentially, increasing the temperature reduces the fluid viscosity (Doederer et al., 2014) and tightens the membrane structure, and it therefore enhances the rejection and the water

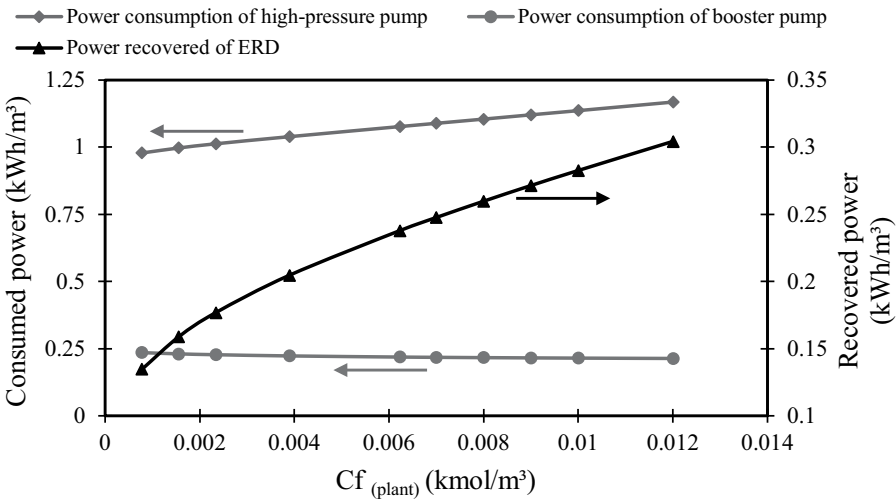


FIGURE 9.43 The effect concentration on the consumed and recovered powers.

(Adapted from Al-Obaidi et al., 2019b)

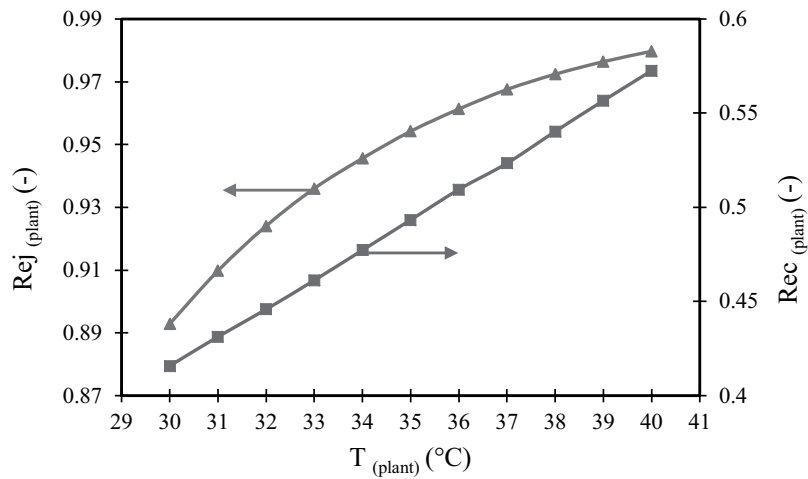


FIGURE 9.44 The effect of feed temperature on the plant rejection and recovery rate. (Adapted from Al-Obaidi et al., 2019b)

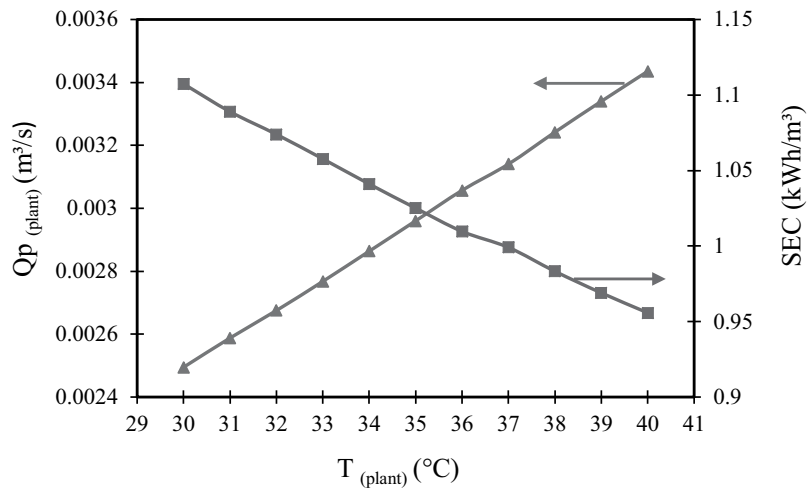


FIGURE 9.45 The effect of feed temperature on the product flow rate and specific energy consumption. (Adapted from Al-Obaidi et al., 2019b)

flux. Indeed, working at a high-temperature medium increases the water and solute transport parameters. It also increases water permeation through the membrane and causes a slight increase in the rejection parameter (Figure 9.44). The impact of feed temperature variation on the total permeate flow rate is depicted in Figure 9.45. This shows an increase of 37.7% in the total permeate flow rate. Additionally, the feed temperature increase causes an SEC reduction of 13.7%.

This is why it is highly recommended to run the process at high temperatures to maintain the process at the lowest *SEC*.

The results described previously have demonstrated a clear picture of the process performance against the variation of the operating conditions. This study has in fact followed the same steps as Sundaramoorthy et al. (2011), where an individual spiral wound RO process, with a wide range of operating conditions and $2.583\text{E-}4\text{ m}^3/\text{s}$ of feed flow rate, $6.226\text{E-}3\text{ kmol}/\text{m}^3$ of concentration, 13.58 atm of pressure, and $31\text{ }^\circ\text{C}$ of temperature, was used. $2.583\text{E-}4\text{ m}^3/\text{s}$ of feed flow rate was therefore multiplied by 30, as there are 30 membrane modules in the first stage.

The simulation results showed that the multi-stage RO process has enhanced the total recovery, rejection, and energy consumption by about 39%, 19%, and 37%, respectively. These results compare well to those of Sundaramoorthy et al. (2011), and which were obtained by an individual spiral wound RO process at similar operating conditions. They reported 22% recovery rate, 83% chlorophenol rejection rate, and $2.03\text{ kWh}/\text{m}^3$ of energy consumption, while Al-Obaidi et al. (2019b) reported 30.68% total recovery rate, 91.48% rejection, and $1.28\text{ kWh}/\text{m}^3$ energy consumption.

9.8 DESIGN AND OPTIMISATION OF THE MEMBRANE ELEMENT OF A SPIRAL WOUND RO PROCESS FOR DIMETHYLPHENOL REMOVAL FROM WASTEWATER AT LOW ENERGY CONSUMPTION

Minimising the total energy consumption of any industrial process is one of the main approaches used to maximise the profitability of operation, whereby the emission of gases such as CO_2 is acceptable. Any method for keeping the energy consumption to a strict minimum is therefore the target for many industrial applications. To this extent, several attempts can be found in the open literature to do this for RO processes.

High permeability membranes, using high-efficient energy recovery devices with optimised process parameters, have been successfully manufactured that reduce the energy consumption to an acceptable level. This challenge still exists. To this extent, a few researchers have explored the optimisation of membrane design parameters to reduce the energy consumption required in an RO process for the removal of phenolic compounds from wastewater.

Al-Obaidi et al. (2017b) studied the possibility of reducing the energy consumption and simultaneously maximising the dimethylphenol removal from wastewater by carefully manipulating the membrane design parameters, including membrane length, width, and feed channel height of an individual membrane element of spiral wound RO process (membrane type HM4040-LPE). This is achieved by altering the membrane dimensions, in line with the manufacturer's membrane specifications, as presented in Table 9.4, with the set of operating conditions of $6.548\text{E-}3\text{ kmol}/\text{m}^3$, $2.583\text{E-}4\text{ m}^3/\text{s}$, 13.58 atm, and $31.5\text{ }^\circ\text{C}$ of feed concentration, flow rate, pressure, and temperature, respectively. Al-Obaidi et al. (2017b) developed an innovative simple model (Model X, Chapter 5) to estimate the performance indicators of the RO

process and validate them against the experimental data of Srinivasan et al. (2011). They confirmed the consistency of their model as demonstrated in Table 9.15. The next step they followed is an optimisation study to reach the targeted dimethylphenol rejection and energy consumption values.

The next section outlines the impact of membrane design parameters on the process performance and how they can be optimised for the maximum removal of dimethylphenol at the lowest energy consumption possible.

9.8.1 EFFECT OF MEMBRANE WIDTH AND LENGTH

The membrane width and length were changed at fixed membrane volume, area, and feed channel height of $0.8\text{E-}3\text{ m}$, with the expectation that this would amend the flow patterns and positively impact on the removal of dimethylphenol, permeate recovery, and total energy consumption. This is exactly what happened and is illustrated in Figures 9.46 and 9.47. Increasing the membrane length or decreasing the membrane width actually causes an increase in dimethylphenol rejection. This is attributed to increasing the bulk velocity as a result of increasing membrane width. This, in turn, decreases the dimethylphenol concentration on the membrane wall, therefore limiting the solute flux and improving the rejection. Moreover, increasing membrane width can reduce the pressure drop, which promotes the permeate flux and the total permeate recovery. Interestingly, both the permeate recovery and energy consumption yield an optimum value of membrane width. This resulted in a maximum permeate recovery value and reduced energy consumption. These findings are entirely consistent with those of Karabelas (2014), who confirmed the improvement of recovery with the application of short sheets of membranes.

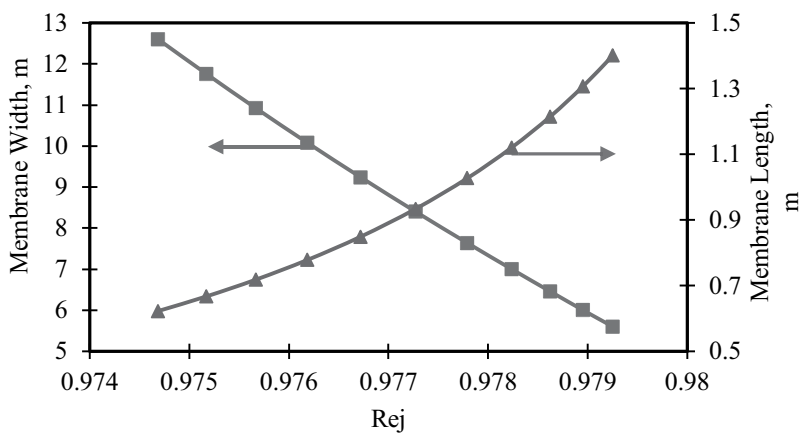


FIGURE 9.46 Effect of membrane length and width at constant membrane area on dimethylphenol rejection.

(Adapted from Al-Obaidi et al., 2017b)

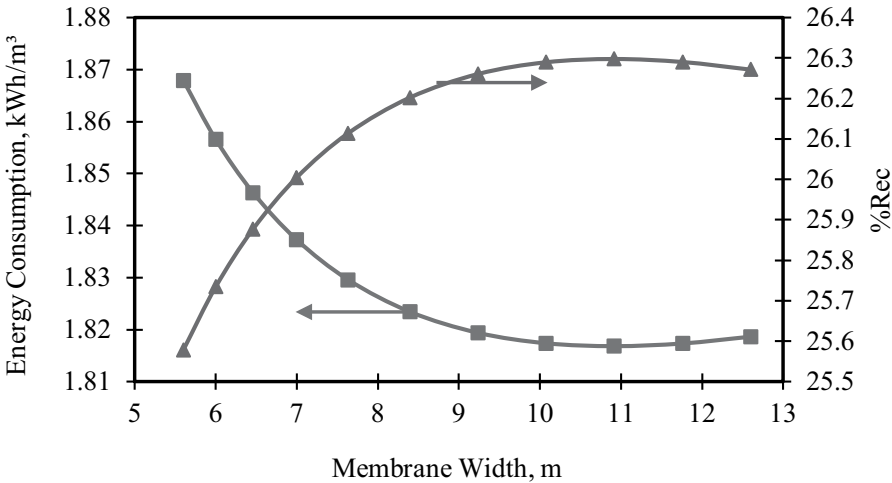


FIGURE 9.47 Effect of membrane width at constant membrane area on energy consumption and total recovery.

(Adapted from Al-Obaidi et al., 2017b)

9.8.2 EFFECT OF FEED CHANNEL HEIGHT

Figure 9.48 illustrates the influence of feed channel height on the rejection of dimethylphenol and the total energy consumption at fixed membrane area and variable membrane volume. The simulation was carried out at the same operating conditions as in the previous section. A reduction of dimethylphenol rejection and an increase in energy consumption were noticed with the increase of feed channel height. This is attributed to the increasing pressure drop with the increasing height of the feed channel, which limits the permeate flux, thus requiring a higher energy consumption. Similar observations were also made by Gu et al. (2017) for a spiral wound RO seawater desalination process.

9.8.3 OPTIMISATION OF MEMBRANE DESIGN PARAMETERS

An optimisation problem was formulated to maximise dimethylphenol rejection at the lowest energy consumption for the specified membrane type HM4040-LPE. A fixed membrane area of 7.84 m² was used, and the optimisation was carried out for different operating conditions of feed concentration, pressure, flow rate, and temperature.

The optimisation problem was formulated as follows:

Max and MinRej, E

L, W, t_f

Subject to: Equality constraints:

Process model: f(x, u, v) = 0

Inequality constraints: 0.5 ≤ L ≤ 1.0

5.0 ≤ W ≤ 15.69

5.93 × 10⁻⁴ ≤ t_f ≤ 10⁻³

Equality endpoint constraint: A = 7.84 m²

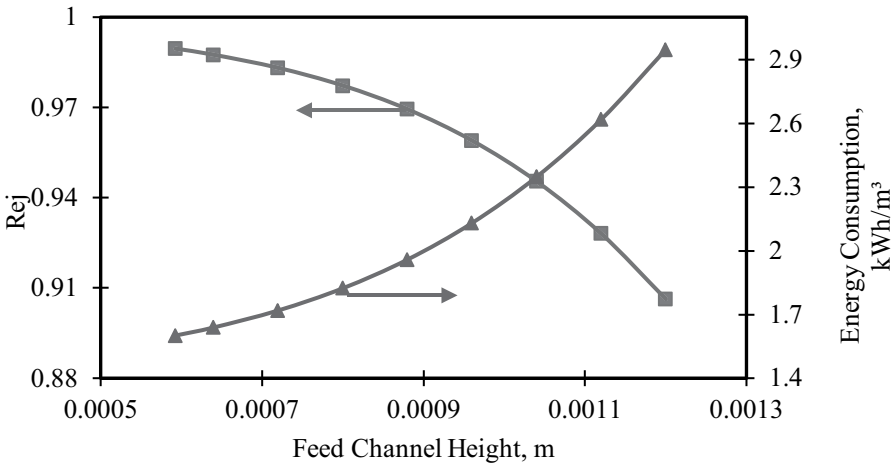


FIGURE 9.48 Effect of feed channel height increase at constant membrane area on dimethylphenol rejection and specific energy consumption.

(Adapted from Al-Obaidi et al., 2017b)

The optimisation resulted in the optimal values of the membrane dimensions of 0.805m as the membrane length, 9.745m as the membrane width, and 5.93E-4 m as the height of feed channel. The optimum reduced value of height of the feed channel can be considered as a feasible and practical option for a spiral wound RO process since wastewater usually has a low concentration of pollutants and therefore a low fouling opportunity. Consequently, the possibility of membrane clogging is low. The optimisation results are presented in Table 9.15 with the maximum rejection values resulting in energy savings between 5.28% and 19.2%, based on the set of operating conditions.

9.9 DESIGN AND OPTIMISATION OF MEMBRANE ELEMENTS OF A MULTI-STAGE RO PROCESS FOR THE REMOVAL OF CHLOROPHENOL FROM WASTEWATER WITH SIGNIFICANT ENERGY SAVINGS

Al-Obaidi et al. (2018d) analysed the influence of varying the membrane design dimensions of membrane elements, including the membrane length, width, and feed channel height, of a multi-stage RO process on the removal of chlorophenol, permeate recovery, and energy consumption. This was originally carried out for two series configurations, with and without energy recovery device and four pressure vessels of one membrane element per each vessel of RO process. The membrane selected is HM4040-LPE and its specification is presented in Table 9.4.

The model developed by Al-Obaidi et al. (2017b) (Model X, Chapter 5) was calibrated and used in this study to satisfy the calculation of energy consumption, for both with and without an ERD.

TABLE 9.15
Model Validation, Simulation, and Optimisation Results

TABLE 9.15 Model Validation, Simulation, and Optimisation Results																			
No	P _{bin} (atm)	T (°C)	C _f × 10 ³ (kmol/m ³)	Q _f × 10 ⁴ (m ³ /s)	Validation section				Optimisation section										
					P _{bout} (atm)	%Error	Q _f × 10 ⁴ (m ³ /s)	%Error	Rej	%Error	Rec	Rej	Specific energy consumption (kWh/m ³)	Non opt.	Opt.	Non opt.	Opt.	% Energy saving	
1	5.83	32.5	0.819	2.166	4.46	4.00	10.2	1.800	1.892	-5.1	0.902	0.932	-3.3	12.65	13.63	0.966	1.626	1.504	7.50
2	7.77	32.5	0.819	2.166	6.31	6.01	4.78	1.670	1.751	-4.8	0.915	0.944	-3.1	19.16	20.40	0.974	1.428	1.340	6.21
3	9.71	32.5	0.819	2.166	8.14	8.01	1.59	1.590	1.610	-1.2	0.927	0.950	-2.5	25.67	27.16	0.978	1.332	1.257	5.62
4	11.64	32.5	0.819	2.166	9.98	10.00	-0.2	1.500	1.471	1.9	0.936	0.955	-2.0	32.08	33.87	0.981	1.277	1.209	5.36
5	13.58	32.5	0.819	2.166	11.8	12.00	-1.7	1.370	1.333	2.70	0.942	0.958	-1.7	38.46	40.58	0.983	1.243	1.177	5.28
6	7.77	31.5	6.548	2.166	6.13	5.97	2.56	1.828	1.850	-1.2	0.952	0.963	-1.1	14.59	17.35	0.982	1.878	1.575	16.1
7	9.71	31.5	6.548	2.166	7.96	7.96	0	1.750	1.730	1.14	0.962	0.969	-0.7	20.13	23.59	0.985	1.699	1.448	14.7
8	11.64	31.5	6.548	2.166	9.97	9.94	0.23	1.641	1.611	1.82	0.970	0.973	-0.3	25.62	29.76	0.987	1.600	1.376	14.0
9	13.58	31.5	6.548	2.166	11.62	11.94	-2.7	1.575	1.494	5.14	0.973	0.976	-0.3	31.02	35.90	0.989	1.540	1.330	13.6
10	5.83	31	1.637	2.33	4.34	3.85	11.3	2.010	2.081	-3.5	0.919	0.934	-1.6	10.68	11.96	0.966	1.926	1.714	11.0
11	7.77	31	1.637	2.33	6.19	5.85	5.5	1.894	1.946	-2.7	0.935	0.946	-1.1	16.48	18.13	0.974	1.663	1.507	9.34
12	9.71	31	1.637	2.33	8.02	7.85	2.13	1.794	1.812	-1.0	0.943	0.953	-1.0	22.23	24.29	0.978	1.538	1.406	8.59
13	11.64	31	1.637	2.33	9.86	9.84	0.23	1.684	1.679	0.29	0.949	0.957	-0.8	27.94	30.41	0.980	1.467	1.346	8.24
14	13.58	31	1.637	2.33	11.68	11.83	-1.3	1.594	1.548	2.88	0.953	0.961	-0.8	33.56	36.52	0.982	1.423	1.308	8.11
15	5.83	31	2.455	2.33	4.29	3.84	10.3	2.022	2.094	-3.5	0.917	0.940	-2.5	10.13	11.59	0.970	2.030	1.768	12.9
16	7.77	31	2.455	2.33	6.14	5.84	4.82	1.907	1.963	-2.9	0.928	0.952	-2.6	15.75	17.68	0.977	1.736	1.546	10.9
17	9.71	31	2.455	2.33	7.97	7.84	1.61	1.815	1.832	-0.9	0.944	0.959	-1.6	21.37	23.77	0.981	1.598	1.437	10.1
18	11.64	31	2.455	2.33	9.81	9.83	-0.2	1.707	1.702	0.29	0.950	0.963	-1.3	26.95	29.80	0.984	1.521	1.374	9.66
19	13.58	31	2.455	2.33	11.64	11.82	-1.6	1.607	1.574	2.05	0.956	0.966	-1.0	32.44	35.83	0.985	1.473	1.333	9.48

20	9.71	29	4.092	2.583	7.8	7.59	2.66	2.113	2.146	-1.5	0.953	0.954	-0.1	16.92	19.93	0.979	2.023	1.714	15.3
21	11.64	29	4.092	2.583	9.61	9.57	0.37	2.070	2.027	2.07	0.958	0.958	-0.1	21.52	25.18	0.982	1.904	1.626	14.6
22	13.58	29	4.092	2.583	11.47	11.56	-0.8	1.971	1.909	3.14	0.965	0.962	0.3	26.09	30.44	0.984	1.831	1.569	14.3
23	5.83	31.5	6.548	2.583	4.08	3.61	11.6	2.337	2.395	-2.5	0.946	0.952	-0.6	7.28	8.99	0.975	2.823	2.281	19.2
24	7.77	31.5	6.548	2.583	5.93	5.59	5.60	2.253	2.273	-0.8	0.954	0.964	-1.0	12.00	14.26	0.982	2.282	1.916	16.0
25	9.71	31.5	6.548	2.583	7.75	7.59	2.05	2.170	2.150	0.92	0.963	0.970	-0.8	16.76	19.56	0.985	2.040	1.746	14.4
26	11.64	31.5	6.548	2.583	9.57	9.57	0	2.090	2.028	2.96	0.969	0.974	-0.5	21.48	24.82	0.987	1.906	1.649	13.5

(Adapted from Al-Obaidi et al., 2017b)



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9.9.1 DESCRIPTION OF THE RO PROCESS AND FEED CHARACTERISTICS

The proposed two configurations of RO process are schematically presented in Figure 9.49 as A and B of three stages and four pressure vessels connected in series in a 2:1:1 ratio. Each pressure vessel contains a spiral wound module of membrane type Ion Exchange, India, of 7.845 m². This is basically designed as a retentate reprocessing scheme. The designs of configurations A and B are the same, except that an ERD and booster pump are used in configuration B. A high-pressure pump of maximum 20 atm was used to raise the pressure of the feed delivered to the first stage. The ERD was used to absorb the energy from the high-pressure retentate stream and transfer it into the low-pressure stream. Also, a booster pump was used to raise the pressure of the split feed stream to the high-pressure pump.

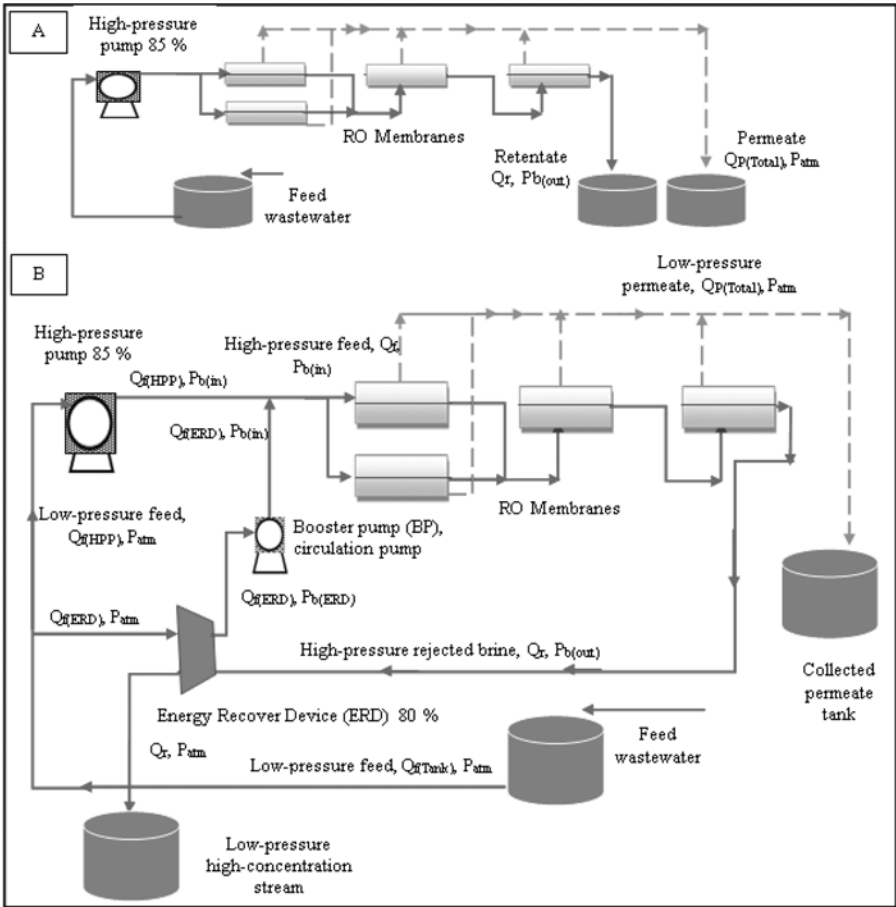


FIGURE 9.49 Schematic diagram of configurations A and B of the RO process.

(Adapted from Al-Obaidi et al., 2018d)

9.9.2 IMPACT OF MEMBRANE DIMENSION ON THE PROCESS PERFORMANCE

The impact of simultaneously changing the membrane length and width for each module in configurations A and B, as per the manufacturer dimensions, at a fixed area (7.845 m²) and a feed channel height (0.8E-3 m) for the removal of chlorophenol from wastewater, permeate recovery, and energy consumption was studied. The operating conditions were 6.226E-3 kmol/m³ feed concentration, 15 atm, 5.166E-4 m³/s feed flow rate, and 31 °C temperature. Figures 9.50 and 9.51 show the influence of a 5% step increase in the membrane width on the removal of chlorophenol and permeate recovery as well as the total energy consumptions of configurations A and B.

There is a clear decrease of chlorophenol rejection when the membrane width increases because of an increase in the permeate recovery. Increasing the membrane width essentially reduces the membrane length, which reduces the average pressure loss and raises the water flux. In this respect, Lomax (2008) affirmed that a longer width of sheets, but with a shorter length, can enhance the permeate recovery. Also, an increase in the membrane width yields a decrease in energy consumption for both configurations A and B, with a considerably better performance for B. Increasing the membrane width results in a 5.18% decrease in rejection, 5.26% growth in permeate recovery, and a reduction of energy consumption of 13% and 5% for configurations B and A with and without an ERD, respectively. It can therefore be said that configuration B offers a higher energy savings despite having an insignificant reduction in the chlorophenol rejection.

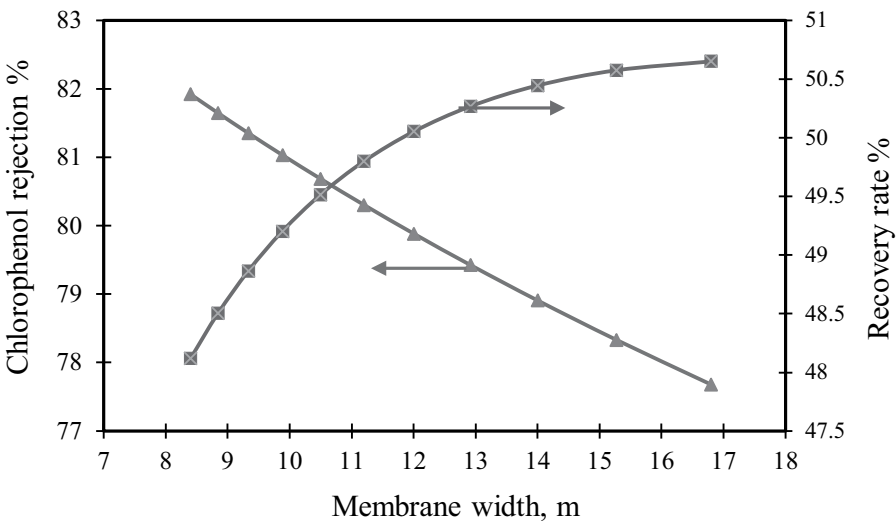


FIGURE 9.50 Influence of increasing membrane width at fixed membrane area and volume on chlorophenol rejection and permeate recovery.

(Adapted from Al-Obaidi et al., 2018d)

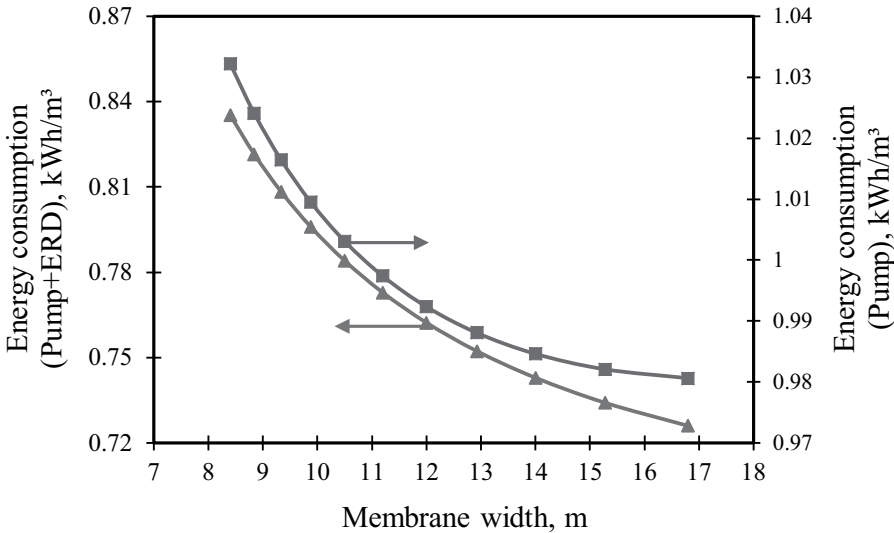


FIGURE 9.51 Influence of increasing membrane width at fixed membrane area and volume on total energy consumption of configurations A and B.

(Adapted from Al-Obaidi et al., 2018d)

9.9.3 IMPACT OF CHANGING THE HEIGHT OF THE FEED CHANNEL

The impact of feed channel height variation on the removal of chlorophenol, permeate recovery, and energy consumptions of configurations A and B are illustrated in Figures 9.52 and 9.53, respectively. The simulations were carried out at fixed membrane area and variable module volume.

Figure 9.52 shows the reduction of chlorophenol rejection and permeate recovery when increasing the height of the feed channel. This causes an increase of the energy consumption when used with and without an ERD, as represented in Figure 9.53. Increasing the height of the feed channel might cause an increase in the pressure drop, and this can reduce the water flux through the membranes and can ultimately decrease the chlorophenol removal. The variation of the feed channel height from 0.5E-3 to 1E-3 m causes a decrease in the chlorophenol rejection and permeate recovery of 25.31% and 30.39%, respectively. The same variation causes an increase of energy consumption of 43.26% and 37.24% for configurations A and B, respectively.

9.9.4 IMPACT OF MEMBRANE AREA

This section investigates the impact of increasing the membrane area by 50% of all the RO modules of configurations A and B on the performance of the process for removing chlorophenol from wastewater. The base area was that of the actual membrane area of 7.845 m², which was incrementally increased to 11.768 m². The

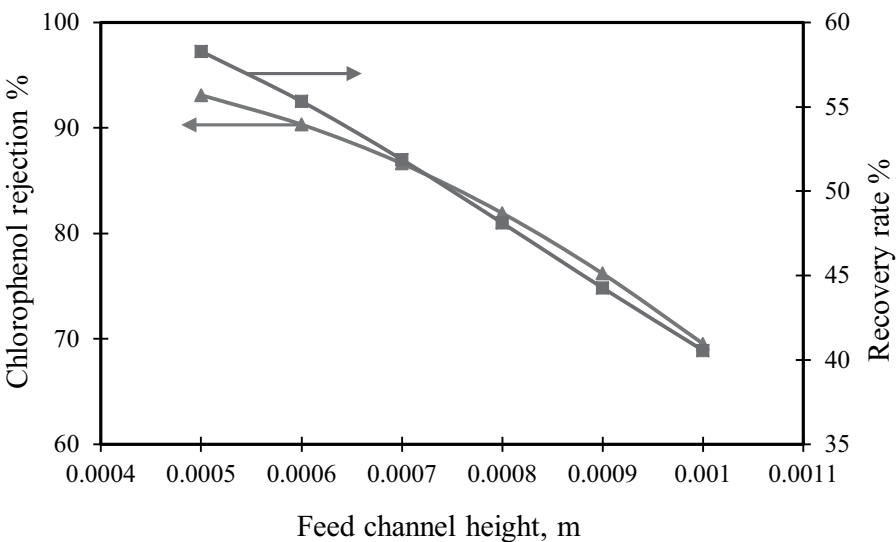


FIGURE 9.52 Influence of increasing feed channel height at fixed membrane area and variable module volume on chlorophenol rejection and permeate recovery.
(Adapted from Al-Obaidi et al., 2018d)

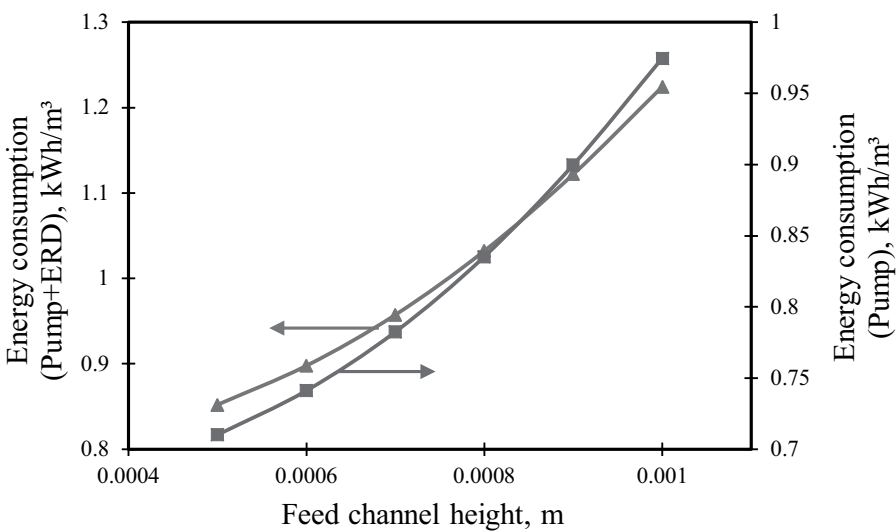


FIGURE 9.53 Influence of increasing feed channel height at fixed membrane area and variable module volume on the total energy consumption of configurations A and B.
(Adapted from Al-Obaidi et al., 2018d)

simulation is carried out at the same operating conditions mentioned in the earlier section. Two options were considered as follows:

- 1. Increase the membrane length by 50% with an incremental increase of 10% at fixed original membrane width and feed channel height of 8.4 m and 0.8E-3 m, respectively.
- 2. Increase membrane width by 50% with an incremental increase of 10% at fixed membrane length and feed channel height of 0.934 m and 0.8E-3 m, respectively.

Figure 9.54 shows a reduction of 3% in the chlorophenol rejection when the membrane length increases by 50% from 0.934 m to 1.4 m. However, a decrease of 6.58% in the chlorophenol rejection is noticed when the membrane width is increased by 50% from 8.4 to 12.6 m. On the other hand, an increase in permeate recovery of 30.90% and 39.76% is noticed when the membrane length and width, respectively, are increased. It is therefore fair to expect that increasing the membrane area by increasing the length or width actually reduces the energy consumption while improving the permeate recovery. Figure 9.55 shows a considerable drop in the energy consumption when the membrane area is increased in both the two options tested. Specifically, decreases of 23.6% and 28.44% are confirmed for configurations A, by increasing the membrane length and width, respectively. Moreover, a decrease of 15.81% and 24.09% are confirmed for configurations B, by increasing the membrane length and width, respectively.

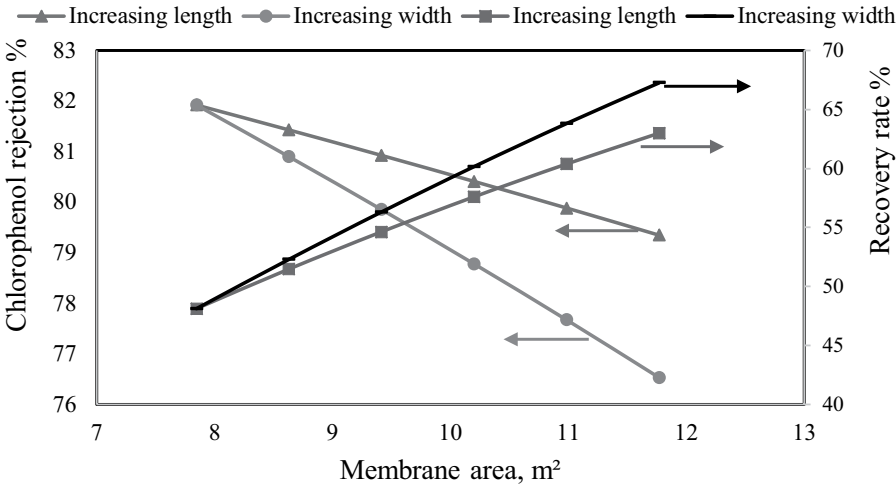


FIGURE 9.54 Influence of 50% increase in membrane area caused by two options of increasing membrane length and increasing membrane width on chlorophenol rejection and permeate recovery.

(Adapted from Al-Obaidi et al., 2018d)

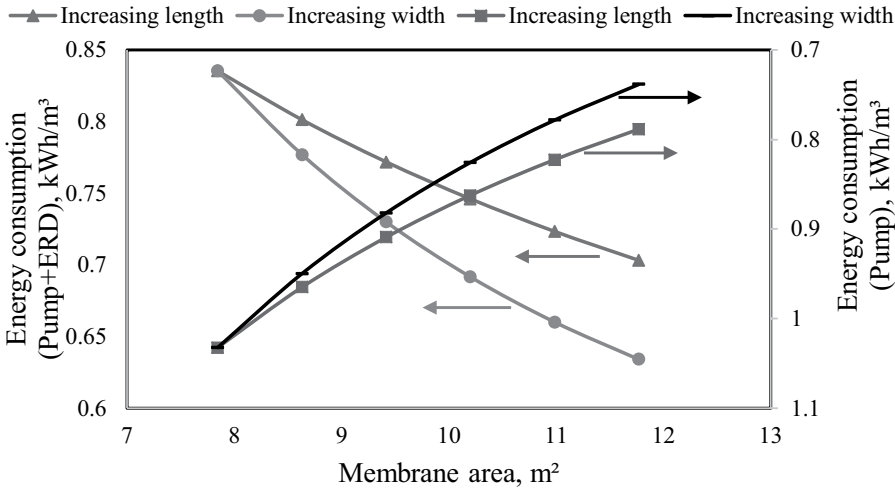


FIGURE 9.55 Influence of 50% increase in membrane area caused by two options of increasing membrane length and increasing membrane width on energy consumption of configurations with and without ERD recovery.

(Adapted from Al-Obaidi et al., 2018d)

9.9.5 IMPACT OF INCREASING THE MEMBRANE AREA BY SIMULTANEOUSLY INCREASING MEMBRANE LENGTH AND WIDTH

This section investigates the impact of increasing the membrane area by 50% of all the RO modules of configurations A and B by simultaneously increasing the membrane length and width. The base membrane area is 7.845 m² and the feed channel height is 0.8E-3 m. The simulation is carried out using the same operating conditions mentioned in the earlier section.

Figure 9.56 shows a reduction of chlorophenol removal of 4.82% and a substantial increase of permeate recovery of 36.42% when area is increased by 50%. Moreover, an energy consumption decrease of 20.97% and 26.69% for configurations A and B, respectively, can be seen in Figure 9.57 for the same increase of membrane area.

When the membrane area is increased by 50% by increasing the membrane width at fixed length and feed channel height, a considerable volume of energy is saved. This increase also yields better results than when the membrane length and width are increased simultaneously for both configurations, with and without an ERD.

9.9.6 OPTIMISATION OF RO PROCESS CONFIGURATIONS WITH AND WITHOUT AN ERD

Al-Obaidi et al. (2018d) presented a multi-objective optimisation to minimise the energy consumption and maximise the removal of chlorophenol for the set of operating conditions of 6.226E-3 kmol/m³, 15 atm, 5.166E-4 m³/s, and 31 °C. The decision variables of the optimisation problem are the membrane length, width, and feed

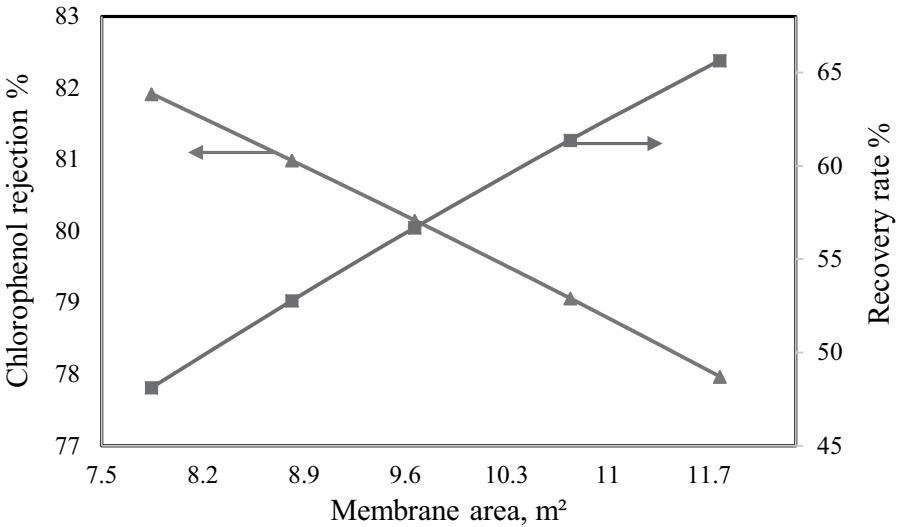


FIGURE 9.56 Influence of 50% increase in membrane area caused by simultaneous increase of membrane length and width on chlorophenol rejection and permeate recovery. (Adapted from Al-Obaidi et al., 2018d)

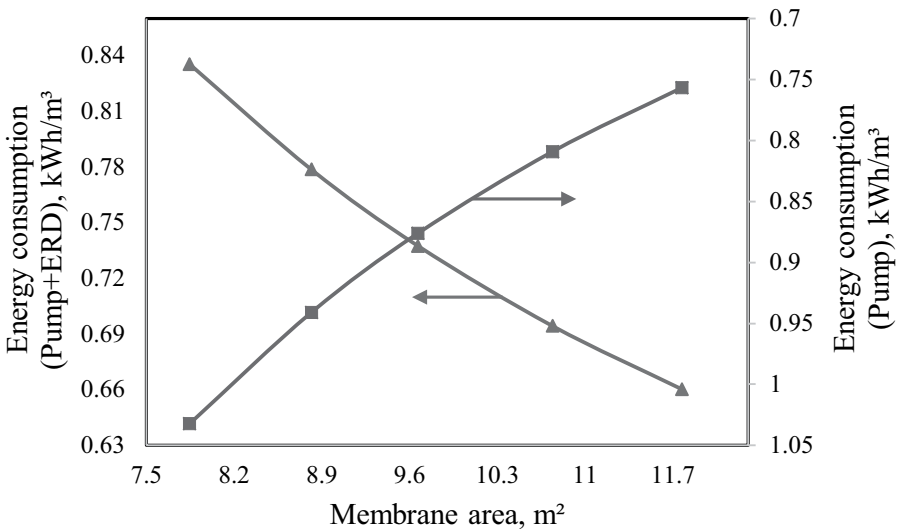


FIGURE 9.57 Influence of 50% increase in membrane area caused by simultaneous increase of membrane length and width on energy consumption of configurations with and without ERD. (Adapted from Al-Obaidi et al., 2018d)

TABLE 9.16
Upper and Lower Limits of Control Variables

Parameter	Lower limits, m	Upper limits, m
Membrane length	0.5	1.4
Membrane width	8.4	12.6
Feed channel height	0.001	0.0005

(Adapted from Al-Obaidi et al., 2018d)

channel height, which are optimised within upper and lower bounds as shown in Table 9.16. The membrane area of 7.845 m² was fixed as a constraint.

The optimisation problem was formulated as follows:

- Given: operating feed parameters and module specifications.
- Optimise: membrane dimensions.
- Minimise: the total energy consumption.
- Maximise: the chlorophenol rejection.
- Subject to: equality (process model) and inequality constraints (linear bounds of optimisation variables).

The optimisation problems can be represented mathematically as:

Min

Max

T. E. C. 1 and T. E. C. 2

$Rej_{(Total)}$

L, W, t_f

Subject to:

Equality constraints:

Process model: $f(x, u, v) = 0$

$A = 7.845m^2$

Inequality constraints:

$L^L \leq L \leq L^U$

$W^L \leq W \leq W^U$

$t_f^L \leq t_f \leq t_f^U$

The energy consumption of configuration A is denoted as T.E.C.1 and that of configuration B as T.E.C.2. Table 9.17 shows the optimisation results of the two proposed configurations A and B in terms of minimum values of energy consumption and maximum values of rejection, together with optimum values of membrane length, width, and feed channel height for each stage.

The results of Table 9.17 confirm the importance of selecting special dimensions of stage 2 membrane length, width, and feed channel height compared to stages 1 and 3. This is critical for guaranteeing the maximum permeate flux and permeate recovery. This is, in fact, the consequence of amalgamation of two high-concentration

TABLE 9.17
Optimisation Results of Multi-Stage RO Process of Two Configurations A and B

Stage no.	Optimised membrane dimensions, m		Minimum total energy consumption, kWh/m ³		Maximum chlorophenol rejection % Rej _(Total)	Total water recovery % Rec _(Total) (calculated)
	Length, L	Width, W	Feed channel height, t _f	T.E.C.1 (configuration A with pump)	T.E.C.2 (configuration B with pumps+ERD)	
1	1.40	5.60	0.5E-3			
2	1.09	7.18	0.5E-3	0.93	0.81	53.6
3	1.40	5.60	0.5E-3			

(Adapted from Al-Obaidi et al., 2018d)

streams of stage 1, making a single high feed flow rate stream into stage 2 pressure vessel. Thus, the selection of a larger membrane width plays an important part in the feed flow rate drop (note, increasing the width of membrane for the same flow rate would reduce the bulk velocity inside the module compared to a smaller width membrane) along the whole section, as it produces a higher permeate flux with some energy savings. More importantly, the energy consumption of configurations A and B exhibited a considerable decrease of 60.32% and 54.42%, respectively, when compared to the optimum results of Sundaramoorthy et al. (2011) (the study was carried out in an individual membrane of RO process). Essentially, the permeate recovery realised in both configurations is 53.55%, which is higher than the maximum recovery of 22% reported by Sundaramoorthy et al. (2011). Additionally, the chlorophenol rejection was 93.5% compared to 83% as reported by Sundaramoorthy et al. (2011).

9.10 CONCLUSIONS

This chapter has explored the latest advanced energy-efficient designs of multi-stage spiral wound RO processes for the removal of highly toxic pollutants from industrial wastewater.

It has discussed the merits and feasibility of several complex designs including a two-stage/two-pass RO configuration, a smart permeate reprocessing methodology, a primitive design of a multi-stage RO process based on the retentate-permeate reprocessing approach, and a permeate and retentate recycling in a multi-stage and multi-pass RO process, which has yielded a higher removal of pollutants at low energy consumption.

The optimisation membrane design parameters within the allowable operational limits has yielded a higher removal of highly toxic compounds at an acceptable energy consumption, and one that is better than the original pilot-scale study. Moreover, the use and impact of several energy recovery options have also been discussed on the multi-stage RO process, together with the influence of operating conditions on the energy consumption. The RO configuration of permeate reprocessing technique has clearly achieved the highest removal of NDMA.

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10 Economic Aspects of RO Process for Wastewater Treatment

10.1 INTRODUCTION

The removal of organic micropollutants from industrial effluents is carried out using a wide range of treatment methods such as UV irradiation, organic solvent extraction, steam distillation processes, adsorption, and membrane technology. Both economic and technical objectives are important factors when implementing membrane technology for wastewater treatment. The main factors which affect the product unit cost include the quantity and quality of the produced stream, the process design and operating conditions, energy, the wastewater disposal, the plant site, and finally a variety of economic aspects (Van der Bruggen et al., 2001). The membrane flux is the most influential factor for determining application costs in terms of the required pressure, energy, and plant size. The annualised treatment cost and specifically the associated water production cost are critical for evaluating any technology and assessing its feasibility. In this respect, the total annualised cost for water production includes the summation of annualised investment and operational costs. A detailed economic comparison of the treatment methods begins with a guesstimate value of the total treatment cost. In this respect, the reverse osmosis (RO) process has proved to offer a significant reduction in the cost of potable water from seawater desalination compared to traditional and thermal treatment processes. More importantly, the RO process also has a low consumption of energy compared to thermal separations. The cost estimation for membrane technologies is not trivial, especially when applied to the removal of organic compounds from wastewater. The overall operating cost of a high-quality RO-based water production system for wastewater treatment, using a chemical treatment process in isolation or in combination with other treatment processes, can be reduced significantly using appropriate optimisation tools. Such costs must also take into account the various stringent environmental regulations. This is why there is an urgent need to thoroughly understand and optimise all the economic aspects of membrane technology.

A number of economic functions, which have been developed for seawater desalination, can be readily applied to RO wastewater treatment. This chapter provides a detailed review of all aspects of the cost information for RO water and wastewater treatment. It includes the state of the art on RO economics for water desalination, with a particular emphasis on wastewater treatment.

10.2 STATE OF THE ART OF ECONOMIC ASPECTS OF WATER AND WASTEWATER RO TREATMENT PROCESSES

The optimisation of the total water production cost in an RO process-based water treatment is a key aspect of this separation technology and has attracted the attention of many researchers. This total cost, especially for an RO process, relies heavily on several parameters, including capital costs, operating costs (energy, chemical, labour, waste disposal, and facility management costs), maintenance costs, and the underlying interest rate. Figure 10.1 shows the main categories of total annualised costs, capital costs, and operation costs (Younos, 2005; Khayet, 2013). In this respect, the capital cost (fixed cost) includes all the expenses incurred before the commercial use of the plant and during the construction of the project, which include direct and indirect capital costs. These are associated with planning, designing, and constructing costs. Operation and maintenance costs are associated with all the expenditure throughout the plant lifecycle and essentially represent the ongoing costs for operating the plant. Such costs also include direct and indirect (overhead) costs. More specifically, operation and maintenance costs include membrane replacement, energy, chemicals, and labour (Banat and Jwaied, 2008; Elazhar et al., 2009; Lapuente, 2012). Capital, operation, and maintenance costs are relatively affected by other parameters, including feed water concentration, plant capacity (total permeate flow rate), construction year, energy cost, infrastructure requirements, region, operating conditions, permeate requested quality, module and plant design, and lifetime events (Jirjis and Luque, 2010; Loutatidou et al., 2014).

Overall, the total annualised cost (TAC) is the summation of annualised capital cost and the annual operation and maintenance cost. The water production cost can be calculated by dividing the sum of the annualised capital costs and the annual operation and maintenance costs by the average annual water production volume. It can therefore be said that the water production cost is highly sensitive to any change in the total production volume. The water production cost is a useful tool for comparing similar projects of different sizes. Poullikkas (2001) investigated the contribution of several parameters on the water production cost of RO seawater desalination, as demonstrated in Table 10.1. It is noticeable that both capital costs and energy costs are the major contributors for the production water in an RO seawater desalination scheme. A range of 15% to 30% can be assumed for operation and maintenance costs, given the plant size. Any reduction therefore of such costs would help reduce the overall water production cost. Several attempts have been used to reduce capital and operation costs. They include the enhancement of water permeation of membrane elements (increasing the membrane area per unit volume), improved membrane life, capacity to work at high operating pressures, the use of low-cost membranes, and the development of a highly efficient pumping system. Other attempts have been based on the additional use of energy recovery devices (ERD), which contribute to lowering the total energy consumption.

Overall, the optimisation of design and operation as well as improvements made in pretreatment processes represent two critical factors for reducing water production costs and increasing plant capacity (Ghaffour et al., 2013). With all the several attempts available in the literature, it is fair to say that the overall water production cost of both RO seawater desalination and wastewater treatment has indeed come

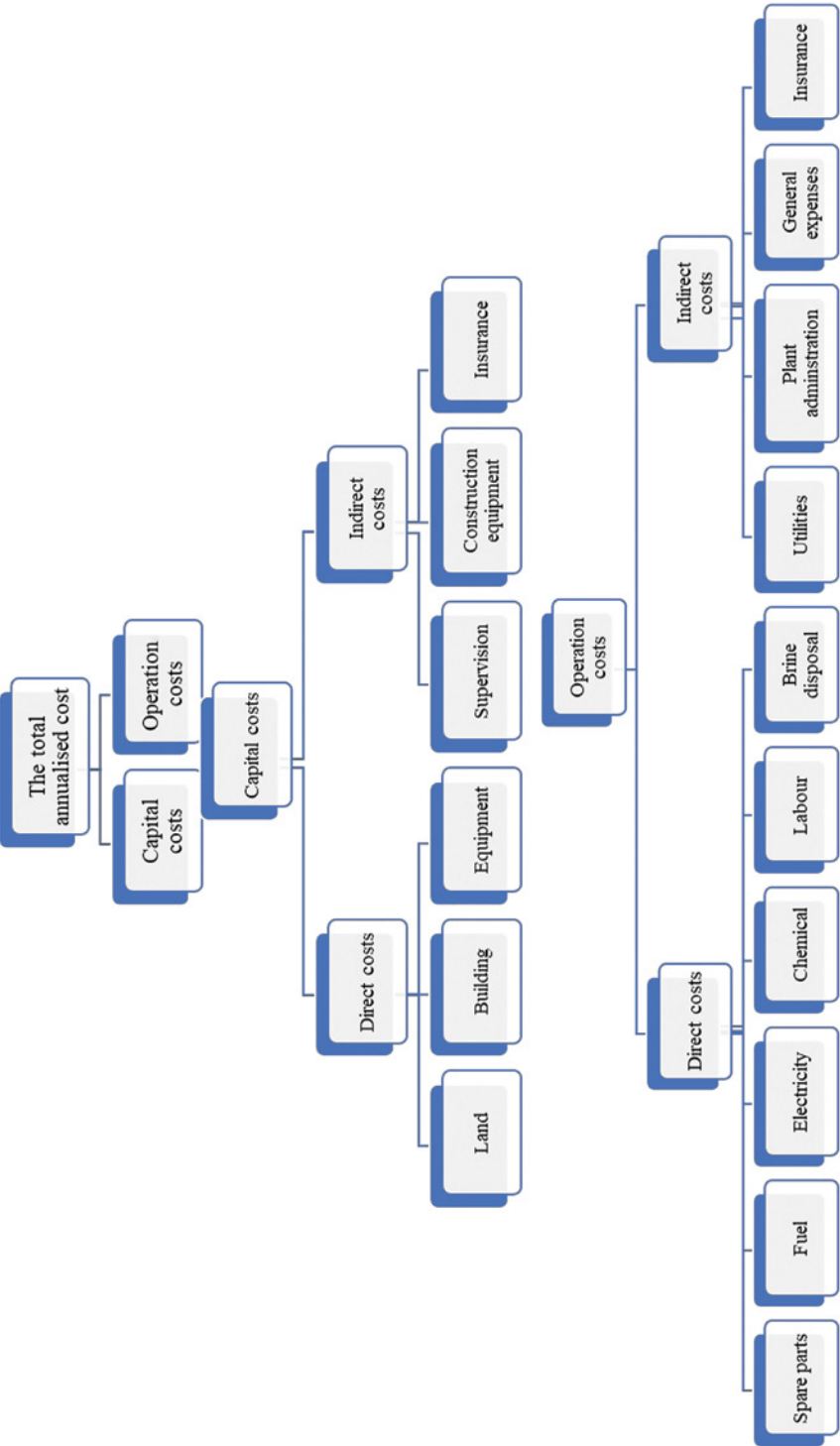


FIGURE 10.1 Categories of total annualised cost, capital costs, and operation costs.

TABLE 10.1
Contributions of Several Cost Parameters on the Freshwater Production Cost

Parameter	Contribution ratio%
Capital cost	30–50
Energy cost	30–50
Operating and maintenance cost	15–30

(Adapted from Poullikkas, 2001)

down over the past few years. This overall cost depends on the feed water, in that it is lower for lower concentration.

The operational cost varies with time due to the change in energy price and expected inflation. Overall, the estimation of permeate production cost in an RO water treatment can be carried out using cost function models (or correlations). Many such models are available with published historical data in various membrane applications. Generally, specific engineering decisions for the process operation or plant design can be made as a result of a preliminary estimated water production cost, which is made up as a function of decision variables.

The open literature confirms several simulation and optimisation attempts for estimating water production costs of RO processes in both seawater desalination and wastewater treatment of various plant sizes. However, applying the same to an RO wastewater treatment requires careful attention and is certainly not trivial. In some attempts, researchers used the same chemical cost equation for considering the total feed flow rate of the stream treated.

The interest of developing cost functions to predict the cost investment and water production cost began in 1993, when several researchers developed cost models for water treatment applications. The initial stochastic capital and operating cost model was developed by Pickering and Wiesner (1993) for a low-pressure membranes-based water treatment plant. The model included several correlations of capital and operating cost estimates. The sensitivity analysis carried out showed the importance of the permeate flux as a main indicator of the total cost. This is because it is dependent on the number of membranes used and the plant capacity. The membrane life is equally dependent on the unit volume of water produced. Any increase of the feed flow rate can cause a higher-pressure loss through the membrane, which in turn increases the required energy cost for recycling the concentrated stream. Another important conclusion from previous studies is that the cost of water production in low-pressure membrane technology, used to remove particles and dissolved organic carbon from medium- to high-concentration raw water, is approximately twice that required to treat low-concentration streams such as groundwater or wastewater. Also, the result of the Pickering and Wiesner (1993) study showed that the total cost of system decreases as a result of an increase in the water permeate flux, which corresponds to a decreasing number of membrane modules used.

Owen et al. (1995) analysed the economics of membrane technology for water and wastewater treatment. The results of a batch and continuous mode

low-pressure 5 m³/day pilot plant of hollow fibre RO membranes and a set of cost functions developed were used to estimate the total water production cost. The comparison of different membrane types showed that membrane cost, membrane replacement, and power requirement are key factors in water production costs. This comparison also revealed that the cost of treating secondary effluents for a 2000 m³/day average flow pilot scale was around 20 to 81 pence/m³ based on membrane type.

Malek et al. (1996) presented a comprehensive RO cost model to predict the performance of a large-scale seawater desalination hollow fibre RO plant. The cost analysis study conducted for a single-stage RO process confirmed that the production unit cost is almost 37% of the total capital cost. They found that the production water cost is relatively unresponsive to energy cost fluctuations due to its low contribution to the total operating cost. The most important conclusion was that large-sized RO plants would offer better opportunities for reduced costs. Malek et al. (1996), who also attempted similar studies, neglected labour and maintenance costs.

Voros et al. (1997) developed a comprehensive methodology, which incorporated a mathematical model to estimate the performance of a hollow fibre RO network (membrane module, pump, and ERD) using given cost equations. This methodology was used to synthesise the optimum RO network at minimum total annualised cost for several types of RO membranes. They considered the quantity and quality of water produced in an optimisation platform. This was formulated as a non-linear programming problem for several RO networks and was used to optimise the superstructure at the lowest total annualised cost. Several arrangements of RO modules, pumps, and ERDs were therefore investigated in this study. The total annualised cost included the capital cost of RO modules, pumps, and ERDs, as well as the operating costs of pumping the energy and the absorbed energy of the ERD. Several conclusions were made and include:

- The total production cost is a function of the product flow rate.
- A decrease in the feed concentration results in a reduction in the total annualised cost.
- The product concentration is an important factor for selecting an appropriate RO superstructure.

This methodology can be applied to any type of feed water, albeit with very low concentrations such as wastewater.

Sethi and Wiesner (2000) developed a comprehensive cost model to estimate the capital cost in a low-pressure membrane technology (crossflow ultrafiltration and microfiltration processes). Several correlations were included to measure the influence of water quality, plant capacity, and operating variables on capital cost. They also used several correlations to estimate the capital cost of several major components. The operating cost model developed by Pickering and Wiesner (1993) were incorporated within this model. Despite this research having been conducted in ultrafiltration and microfiltration membrane technologies, it was concluded that the capital cost actually decreases with the plant capacity and is significantly sensitive to process operating conditions, where an increase of operating pressure reduces the capital cost because of the increasing permeate flux.

Poullikkas (2001) developed an optimisation algorithm used to calculate the water production cost for various RO desalination schemes. The capital cost, operation and maintenance costs, and energy consumption were included to obtain the lowest cost of several RO seawater desalination schemes.

The cost model equations developed for nanofiltration (NF) wastewater treatment can be used for an RO wastewater treatment. Van der Bruggen et al. (2001) used a double pass module design of retentate recirculation of nanofiltration membranes to test its capacity for the removal of pesticides, hardness, and nitrates from a ground-water source. The experimental results were used to evaluate the investment cost of an NF facility and determine the product unit cost. The calculation of investment cost included capital, operating, and maintenance costs but ignored land costs using economic functions. The details of the cost model equations are given in Table 10.2.

TABLE 10.2
Cost Model Equations of Van der Bruggen et al. (2001)

Capital cost equations $C_{capital}$ (£)	
Civil investment (£): includes plant building where 30 years of depreciation period is assumed. Q_f in m^3/s , (n is number of membrane module)	$C_{civil} = 862 Q_f + 1239 n$
Mechanical engineering (£): includes cost of pumps, filters, and other utilities where 15 years of depreciation period is assumed	$C_{mechanical} = 3608 Q_f^{0.85} + 908 n$
Electrotechnical costs (£): includes all costs of supplying energy, control, and all electronic components (P is the applied pressure bar)	$C_{electrotechnical} = 1.4 \times 10^6 + 54 P Q_f$
Membrane investments (£): includes membrane cost where 5 years of membrane lifetime and 1000 £ of one membrane module cost are assumed	$C_{membraen} = 1000 n$
Operating cost equations (£)	
Depreciation costs (£): calculates based on investment cost where no interest is assumed	$C_{depreciation} = \frac{C_{civil}}{30} + \frac{1}{15} \left(C_{mechanical} + C_{electrotechnical} + \frac{C_{membraen}}{5} \right)$
Energy cost (£): includes consumed energy to feed the water into the filtration system where 40 Wh/ m^3 for each m^3 is assumed. Also, 0.05 £/kWh is assumed as the electric cost (Δp is the applied pressure difference, bar).	$C_{energy} = \left(\frac{Q_f \Delta P}{energy\ efficiency} \right)$
Chemical cost (£): includes chemical cost of total feed flow rate to be treated	$C_{chemical} = 0.023 Q_f$
Maintenance cost (£): assumed as 2% of the total capital costs	$C_{maintenance} = 0.02 C_{capital}$
Quality control cost (£): assumed as 2% of the total capital costs	$C_{quality\ control} = 0.02 C_{capital}$
Operation of installation (£): assumed as 2% of the total capital costs	$C_{instillation} = 0.02 C_{capital}$

The results showed that the optimal pressure of operation produced the minimum treated water production cost of 0.126 €/m³. This corresponded to 90%–95%, 76%, and 95% range of pesticides, nitrate, and hardness removal, respectively. The same model of Van der Bruggen et al. (2001) was used by Mohammad et al. (2007) to assess the economic aspect of a nanofiltration seawater desalination application. This shows the possibility of using a wastewater cost model for seawater applications despite their being recognised as more expensive than water reuse and reclamation applications.

The economic analysis of a wastewater treatment facility involves many uncertain factors that could complicate the decision-making process. The prediction of construction costs for wastewater treatment facilities, which is essential for the economic assessment of various control regimes, is one of these uncertain factors. In this respect, Chen and Chang (2002) developed a new methodology for determining the construction costs of an industrial wastewater treatment plant using a combined RO process and several industrial processes. They investigated possible uncertainties based on three regression techniques. They then used them to accurately forecast the optimal size of a wastewater treatment plant leading to the lowest construction cost. The higher prediction accuracy was obtained using a fuzzy goal programming technique, which showed the merits of a flexible pattern compared to two other linear regression methods used.

Marcovecchio et al. (2005) used the combination of cost functions and the Kimura-Sourirajan model (an extended model of Kedem and Katchalsky, 1958; Spiegler and Kedem, 1966) (Chapter 5) to estimate the product cost and predict the transport phenomena of the solute and water transport through the hollow fibre RO membrane. This combination was used later to generate a global optimisation algorithm in order to optimise a large-scale hollow fibre RO seawater desalination system. It was then applied to minimising the capital, operation, and maintenance costs. It was concluded that the feed concentration reduction could cause a reduction of the water production cost. However, the model presented by Marcovecchio et al. (2005) did not take into account labour and maintenance costs.

A preliminary economic comparison study was conducted by Côté et al. (2005) to evaluate the water production cost of two RO filtration and ultrafiltration pre-treatment plants. The first one was based on the treatment of secondary sewage water while the second plant was based on treating seawater. The study confirmed that the capital and operating costs of an RO seawater process are twice the costs of an RO wastewater treatment process. This was attributed to the use of higher operating pressure and feed flow rate in the seawater desalination process compared to the wastewater treatment. One conclusion resulting from this study is that when the permeate flux (and accordingly total recovery rate) is increased up to 50%, it causes a decrease in the water production cost with a gradual increase after 50% water recovery. Also, increasing the RO membrane life reduces the total water cost.

A linear cost model was developed by Sipala et al. (2005) to estimate the unit production costs of treated wastewater for a wide range of treatment processes and reused wastewater. The plant capacity and the level of discharged sewage were taken into consideration for building the cost model. The treatment cost of the related

treatment processes was essentially dependent on several parameters, including environmental rules and wastewater reuse scenarios. A significant variation of water treatment cost was presented in this study.

Gonzalez-Serrano et al. (2005) developed a set of economic functions to estimate the cost of investment, operation, and maintenance of a wastewater treatment plant based on a technical design. This method included investment, operational, and maintenance costs. The method developed was used to assess the performance and cost of several wastewater treatment facilities in seasonally stressed regions. Meanwhile, the impact of the plant size was only included in the cost estimation, which is a limitation of this approach.

Lu et al. (2006) used the mixed integer non-linear programming (MINLP) optimisation problem to minimise the total annualised cost of RO seawater desalination based on a combined model process and cost equations collected from the literature. The optimisation platform considered the annual operating cost and the annualised capital cost. These include energy, membrane cleaning, and replacement costs. The study showed a minimum total annualised cost in line with the optimum RO maintenance schedule.

Dolnicar and Schäfer (2006) compared the economics of two similar RO processes treating different quality effluents of seawater desalination and tertiary wastewater treatment. This study affirmed that the capital cost and tertiary wastewater treatment was about half of the seawater desalination cost. However, the calculation of primary and secondary wastewater treatment facilities was not included. Similarly, the operation and maintenance costs required for high-quality water from an RO seawater desalination plant was twice that of reusing secondary effluents.

Blank et al. (2007) confirmed the need for several actions to reduce the freshwater production cost of both an RO membrane technology and a multi-stage flash thermal technology. Indeed, they reviewed several methods to determine the total production cost.

An economic analysis and optimisation study for three different designs of different membrane types and orientations of membrane system in a wastewater treatment plant capacity of 27 m³/h to treat the discharge of palm oil mill effluent were investigated by Ahmad et al. (2009). The membrane systems were designed as:

- Design A: ultrafiltration (UF) ceramic membranes and RO polymeric membranes.
- Design B: UF polymeric membranes and RO polymeric membranes.
- Design C: two-pass RO polymeric membrane system.

A non-linear optimisation system was carried out for each proposed design to minimise the total treatment cost per cubic metre of palm oil mill effluent and then used to compare the results of the three designs. The costing included the summation of the direct and indirect capital costs and operating costs. Capital costs included the electricity supply, maintenance, chemical, chemical cleaning, and membrane replacement costs. One important conclusion of this study was that the total water recovery had a significant impact on the total treatment cost. Therefore, the optimisation method attained the highest water recovery rate by selecting the highest

operating pressures at the lowest possible crossflow velocity with maintaining the membrane area at minimum value. Furthermore, the total capital cost was dependent on the cost of the membrane system. The membrane replacement cost had the most significant impact on the operating cost. The optimisation method used showed that design C had the lowest total cost per cubic metre of effluent of 7.03 RM/m³ (Malaysian ringgit) compared to 115.11 and 23.64 RM/m³ for designs A and B, respectively. This shows that the system operating at a high membrane pressure and a low membrane unit cost is more promising than the membrane system working at low pressure and high membrane unit cost. Table 10.3 gives a summary of the estimated cost the proposed designs (A, B, and C).

TABLE 10.3
Estimated Breakdown for Designs A, B, and C

Parameter	Design A	Design B	Design C
Direct capital cost (10 ⁶ RM)			
Pretreatment	0.66	0.66	0.66
Membrane system	49.36	6.87	2.43
Framework	0.35	0.26	0.22
Automation and control	0.21	0.18	0.15
Piping, valves, and fittings	0.1	0.05	0.03
CIP and back-flush system	0.98	0.13	0.05
Labour	0.18	0.11	0.07
Total	51.82	8.26	3.61
Indirect capital cost (10 ⁶ RM)	5.16	0.81	0.34
Total capital cost (10 ⁶ RM)	56.98	9.06	3.95
Annualised capital cost (10 ⁶ RM/year)	4.19	0.67	0.29
Operating cost (10 ⁶ RM/year)			
Electrical	0.22	0.22	0.38
Maintenance	0.25	0.04	0.02
Chemical	0.64	0.64	0.64
GAC replacement	0.04	0.04	0.04
Chemical cleaning	0.1	0.02	0.0013
Membrane replacement	11.11	2.48	0.48
Total	12.35	3.43	1.55
Profit gained from fertiliser sales (10 ⁶ RM/year)	0.88	0.88	0.88
Cost per cubic metre (RM/m ³)			
Capital cost	30.81	4.9	2.13
Operating cost	90.77	25.22	11.37
Profit gained from fertiliser sales (10 ⁶ RM/year)	6.47	6.47	6.47
Total cost (RM/m ³)	115.11	23.64	7.03

Exchange rate: 1 USD = 3.5 MYR as of 22 May 2005

(Adapted from Ahmad et al., 2009)

Park et al. (2010) developed a comprehensive cost model package and an RO process simulation model to estimate the construction and operation cost of a seawater RO desalination plant and to predict the total water recovery and solute rejection. The uncertainty around the affordable energy and the randomness of future financial markets were the additional characteristics considered in the economic model. The model developed was applied in a pilot-scale RO system of two configurations of single-stage single-pass (SSSP) and double-stage single-pass (DSSP). A sensitivity analysis was carried out for the uncertain variables.

Hernandez-Sancho et al. (2011) developed a methodology for better understanding the wastewater treatment processes costs. Compared to the models developed in the literature, such as the one developed by Gonzalez-Serrano et al. (2005), they formulated the operating cost function and maintenance cost as a function of the most common variables of the process. These included the impact of efficiency of pollutant removal, the total volume of wastewater treated per year, and the plant lifetime. Various cost functions were developed to predict the operating and maintenance costs for several wastewater treatment plants using numerical data derived from these plants. The cost model used data from 341 wastewater treatment plants in Spain. This study concluded that the consideration of accurate technology, investment costs and effluent quality, and plant operating and maintenance costs were essential for determining the economic feasibility and sustainability of any wastewater treatment facility. It was also found that the plant age and efficiency of removal were fundamental for determining the total annualised cost.

Lu et al. (2012) provided a comprehensive model for a spiral wound RO desalination process to evaluate the total annualised cost of three streams of water sources, which include seawater, brackish water, and regenerated water. In this respect, a multiple feed and product streams RO system was implemented using a synthesised optimisation method. This was essentially based on an MINLP optimisation problem to find the optimum design of the RO process. The optimisation problem was designed to obtain the lowest possible total annualised cost subject to several structural variables and technical constraints. They include the number and type of membrane elements in each pressure vessel, the stream connections, and the operating conditions. The annual operating and capital costs were used to calculate the total annualised cost of the RO process. The annual operating cost primarily contains the energy cost and membrane maintenance cost. However, the cost of buying the membrane modules, pumps, and ERDs was included in the annual capital cost. Lu et al. (2012) did not consider the calculation of labour and disposed costs.

Ochando-Pulido et al. (2013) developed a model to predict the performance of a pilot-scale spiral wound RO process and analyse the production cost for treating an olive mill's wastewater. The secondary treatment includes oxidation, followed by flocculation-sedimentation and RO process as the final treatment step to get rid of the aromatic organic compounds, such as phenols, tannins, and long-chain fatty acids, and inorganic compounds, such as chloride, sulphate, phosphate, copper, and potassium, found in olive oil wastewater. The cost evaluation indicated 0.87 €/m³ and 1.57 €/m³ as the total costs of the RO operation and hybrid process, respectively.

Kumar et al. (2014) developed a novel benchmarking tool of a Water Price Index (WPI) to evaluate the low-pressure membrane module price against three parameters of the membrane permeate flux, probable life (the two key drivers), and efficiency.

The development of WPI helped develop an analytical index to control the water production cost for a long time of operation while retaining high water quality. Simulation results showed that the permeate flux and life expectancy were the most important factors which control WPI. It was found that the cheapest membrane with the highest flux and longest life yields the lowest WPI.

Loutatidou et al. (2014) developed a cost model which can give an accurate estimation of the capital cost of an RO plant. The six key parameters of this model included the cubic metres of water produced per year, feed water type, feed water concentration, location, award year (engineering–procurement–construction contracted year), and the cumulative capacity of the plant. The model was validated against the dataset of large-scale desalination plants in the Gulf Cooperation Council countries and in five southern European countries. The results showed that the plant capacity has a significant relation with the capital cost, while the plant location has a lesser impact. Moreover, the feed concentration does not appear to be an important factor in the capital cost.

Membrane treatment and specifically an RO process is widely used as a reliable separation method in food processing plants such as the dairy industry. It has also been applied to a wide range of wastewater treatment and water reclamation. In this respect, Suárez et al. (2014) used the economic model developed by Sethi and Wiesner (2000) to evaluate the permeate product cost of a low-pressure RO membrane process to treat condensates from an ultra-high-temperature installation in a dairy plant. Also, a parametric sensitivity analysis was carried out in order to investigate critical parameters, which control the profitability of the membrane system used. The main conclusion drawn from this study was that the annualised capital cost contributes to 29.3% of the operation and maintenance costs. The sensitivity analysis affirmed that the profitability could be increased by 48.6% as a result of increasing the recovery rate by 20%. However, an improvement of only 3.3% was noticed for the profitability of a longer membrane lifetime.

Kumar et al. (2015) extended the use of the WPI, as developed by Kumar et al. (2014), from the membrane module to water and wastewater treatment plants of low-pressure membrane technology. This yielded a WPI as a global metric for the cost of water production to be used for comparing the performance of several water and wastewater treatment plants. This study analysed the contribution of capital cost and operating cost on the WPI. Several cases of water and wastewater treatment plants were tested with data available in the literature and showed several benefits of the WPI developed.

A comprehensive optimisation study to minimise the operational cost of an RO seawater desalination plant was carried out by Jiang et al. (2015). They studied the impact of operating conditions such as seawater concentration, temperature, electricity price, and freshwater demand on the operational cost savings of a full-scale RO seawater desalination using a well-developed model. This included both the transport phenomena equations and a set of cost model equations. The optimisation strategy used showed a significant potential of operational cost savings compared to a conventional operation and highlighted the impact of the main operational parameters on the optimal value of operational costs. The methodology used in this study can be efficiently used in an RO wastewater treatment with an expectation of having a lower water cost production.

Papapetrou et al. (2017) carried out a systematic review of freshwater production costs associated with seawater desalination plants, covering research work up to 2017. This review showed the absence of a consistent cost methodology. Many approaches were based on different assumptions, and most methodologies ignored the land costs.

Al-Obaidi et al. (2019) studied the economic capacity of the multi-stage spiral wound RO process, including both retentate and permeate reprocessing in terms of the removal of chlorophenol from wastewater using simulation and optimisation studies. A full mathematical model package was developed by combining two models of spiral wound RO process and several appropriate cost functions. A sensitivity analysis of different parameters was carried out in a simulation study to understand the economic performance of the process. The permeate cost, total annualised cost, and specific energy consumption were minimised in a multi-objective optimisation framework by optimising the operating conditions, which consisted of the operating pressure and the feed flow rate. The model was based on realistic parameters of permeate product cost calculations such as labour and maintenance costs.

10.3 VARIABLES AFFECTING THE WATER PRODUCTION COST OF AN RO WASTEWATER TREATMENT

The total capital cost and therefore the water production cost of an RO wastewater treatment plant is affected by several variables. For instance, the feed water quality is a critical design variable which controls the efficiency of the treatment, including the total rejection and permeate flux. A low wastewater feed concentration with trace organic compounds requires low levels of energy to reject pollutants after the water has permeated through the membrane surface. A much higher energy is required for a high wastewater feed concentration, such as seawater. Such untreated water may contain a high dosage of chemicals, whose fouling propensity and scaling would require further energy. Generally, the presence of trace organic compounds in wastewater would benefit from a combination of treatment processes; however, these can increase pretreatment costs. The membrane lifetime can also be greatly affected by the feed water quality, with further costs being required for membrane replacement.

The plant capacity is another important control variable which can affect the total water production cost due to its close relation with the number and size of plant utilities, such as membranes, pumps, ERDs, and water tanks. It would be fair to say that the economic scale and operation and management costs of a large-scale RO wastewater treatment plant is comparatively lower than that of a small-scale plant. This reduces the product unit cost due to a higher water production quantity despite higher capital and investment costs.

The site specification determining where the membrane plant is located has an effect on the water production cost. The location of the RO plant near to the main effluent streams can reduce the total unit cost due to lower pumping and piping installation costs.

Furthermore, the operating conditions of the feed wastewater can also have a major impact on the total water production cost. For instance, increasing the operating pressure and temperature leads to decreasing the water production cost as a result of increasing water flux through the membranes.

Finally, other variables can also affect the total water production costs, such as water-related political issues, state permits, and strict regulations.

To sum up, there are several important factors which can lessen the water production cost of RO process-based seawater desalination and wastewater treatment. They include:

- The synthesis of advanced RO membrane materials, which can significantly improve the water permeability and solute rejection.
- The efficiency improvement that can be made to pumping and energy recovery devices.
- The combination of RO process in hybrid treatment systems with an advanced and improved pretreatment step can reduce the use of chemicals and thus costs.
- The improvement in the design of the RO process via superstructure optimisation resulting in energy-efficient designs and thus reducing costs.
- The use of large-scale RO plants, where possible, to benefit from the economy of scale and thus reducing water production costs.

10.4 COST EVALUATION OF RO WATER TREATMENT PLANTS

The cost of water production for an RO membrane technology has been steadily decreased from its early commercial introduction due to several improvements. This has happened despite the continuous rise of energy prices.

Sassi and Mujtaba (2012 and 2013) achieved 0.48–1.3 US\$/m³ of water via an MINLP-based superstructure optimisation of an RO desalination processes operating under a salinity range of 15,000 to 50,000 ppm and a seawater temperature range of 15 to 40 °C. This treatment also included boron removal.

Ghaffour et al. (2013) presented a techno-economic review of the water production cost of RO desalination, where the main parameters that affect the water unit cost are thoroughly described for several desalination facilities. This confirmed that the cost of desalinated seawater has been reduced to around 0.5 \$/m³ for a large-scale RO seawater desalination plant, compared to 1.0 \$/m³ for other RO seawater plants working at the same conditions but at different locations. The difference of capital, operating, and maintenance costs in addition to location and subsidies may explain this difference in freshwater price.

Pickering and Wiesner (1993) and Wade and Callister (1996) affirmed that brackish water desalination is cheaper than seawater desalination for the same size of RO scheme. They confirmed specifically that the seawater desalination cost is three to seven times greater than that of brackish water. The total water production cost is reduced from 1.12–1.85 \$/m³ for high-pressure RO desalination plant to 0.41–0.53 \$/m³ for low-pressure RO brackish water (Pickering and Wiesner, 1993).

The optimisation results of Marcovecchio et al. (2005) confirmed a production cost of between 1.01 and 0.79 \$/m³ for a set of seawater concentrations between 42,000 and 36,000 ppm and an operating pressure of around 68 atm. This is comparable to the current estimation of the water product cost, which is within 0.5 \$/m³ for a large-scale RO seawater desalination plant (Ghaffour et al., 2013). These results are

consistent with those of Shemer and Semiat (2017), who confirmed that the cheapest water production cost of seawater RO desalination is 0.5 \$/m³. However, this value can be increased by 2.5% for some other seawater plants of the same design and equipment. The retardation of freshwater production cost can be attributed to several reasons already discussed in earlier sections.

Côté et al. (2005), Dolnicar and Schäfer (2006), and Al-Obaidi et al. (2019) confirmed that the capital costs for a plant producing high-quality water from secondary effluents are almost half the costs of a plant producing fresh water from seawater sources. In this respect, the pretreatment costs, membrane RO cost, and operating and maintenance costs are lower for producing water from a wastewater source. According to the data obtained by Côté et al. (2005), water production costs from RO wastewater and seawater sources are 0.28 \$/m³ and 0.62 \$/m³, respectively. Guo et al. (2014) stated that water production costs from wastewater applications varied between 0.40 and 1.26 \$/m³. This variation is due to the type of wastewater source, whether primary or secondary wastewater, and also the required type of treatment to reuse the wastewater such as direct or indirect potable or non-potable reuse, industrial water, or irrigation. More recently, Al-Obaidi et al. (2019) explored the possibility of reducing the water production cost to 0.21 \$/m³ of high-quality permeate from a multi-stage RO process for removing chlorophenol from wastewater via simulation and optimisation.

10.5 COST ANALYSIS OF RO PROCESS FOR THE PURIFICATION OF OLIVE MILL WASTEWATER

Ochando-Pulido et al. (2013) carried out a thorough study to assess the performance and calculate the cost of an RO process using integrated oxidation and flocculation-sedimentation processes in an olive mill factory. The RO filtration process has been examined in a pilot scale, where a highly hazardous wastewater containing aromatic compounds, inorganic compounds such as chloride, calcium, sodium, magnesium, copper, sulphate, and phosphoric salts of potassium, iron, and organic chemicals such as phenol, tannins, and fatty acids are treated.

10.5.1 RO PROCESS DESCRIPTION

Figure 10.2 shows a schematic diagram of the pilot-scale tangential flow RO process of a 100 L feed tank, centrifugal booster pump, and spiral wound membrane module. The membrane used was a commercial spiral wound thin-film composite manufactured by GE Water and Process Technologies (Minnetonka, MN, USA). The high-concentration stream was recycled back to the feed tank and the high-quality permeate was collected in the product tank.

10.5.2 ECONOMIC ANALYSIS

A simplified economic analysis was performed by Ochando-Pulido et al. (2013) to investigate the water production cost of a 10 m³ feed flow rate of secondary wastewater coming from the oxidation and flocculation-sedimentation processes into the RO process of two spiral wound modules (parallel layout) with an effective individual surface

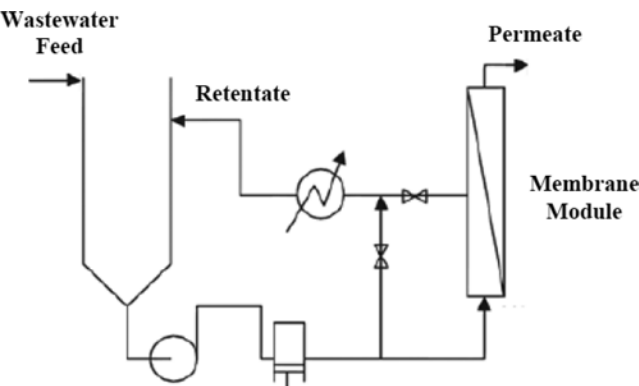


FIGURE 10.2 Schematic diagram of pilot-scale RO process.

(Adapted from Ochando-Pulido et al., 2013)

TABLE 10.4
Cost Analysis of Olive Mill Factory

Item	Cost, €/m ³
Membrane	0.25
Pressure vessel and piping	0.22
Electricity	0.40
Total cost of RO process	0.87
Total cost of three integrated treatment processes	1.57

(Adapted from Ochando-Pulido et al., 2013)

area of 32 m². The cost calculation was based on assuming five years of membrane life-time with an operating time of 10 h per day. The other economic parameters used were:

- The energy cost was set at 0.10 €/kWh.
- The membrane module and pressure vessel costs at 22 €/m² and 380 €, respectively.
- The pumps, piping, and RO process connections were equal to 50% approximately of the pressure vessel costs.
- The capacity space and associated services requires 15% of the total costs.

The final estimated cost calculations of the entire olive mill factory, including two secondary treatment steps and an RO filtration step, are given in Table 10.4. This shows that the total water production cost of the RO process was 0.87 €/m³. However, the total water production cost for the integrated treatment processes was 1.57 €/m³. This corresponds to a high-quality permeate, which contained zero concentration of total suspended solids, phenol, and iron. The operating pressure of the RO process was controlled at medium feed pressure and ambient temperature of 25 bar and 22

°C, respectively. The RO process was maintained for providing a water recovery of 90%, corresponding to 21.1 L/h m² of permeate flow rate.

10.6 COST ANALYSIS OF AN RO PROCESS FOR THE RECLAMATION OF DAIRY WASTEWATER

The model developed by Sethi and Wiesner (2000) to represent the cost of cross-flow ultrafiltration and microfiltration membrane processes was used by Suárez et al. (2014) to provide a basis for the economic assessment and to especially determine the capital expenditure of a low-pressure RO membrane process used to treat condensates from an ultra-high-temperature (UHT) installation in a dairy plant.

10.6.1 RO PROCESS DESCRIPTION

The milk and milk-based products are heated in a high-temperature treatment process to maintain flavours of sterile milk and milk-based products with a shelf life at room temperature of at least six months (Suárez et al., 2014). There are several water specifications to be fed to the boiler to prevent scaling, corrosion, and foams. The main aim of the continuous pilot-scale RO process was to generate a high-quality water from the flash cooler condensate of the UHT process in line with the boiler requirements. The RO plant consisted of two parallel spiral wound thin-film membrane elements type Duratherm HWS 4040 HR membrane (GE Water and Process Technologies, Trevose, PA, USA) and providing an area of 37 m². The plant feed flow rate was 20 m³/h, while the total plant recovery was fixed at 83% and at operating pressure of 1300 kPa.

10.6.2 ECONOMIC MODEL OF SETHI AND WIESNER (2000)

Suárez et al. (2015) used the model proposed by Sethi and Wiesner (2000) to calculate the capital expenditure. This was originally based on non-membrane and membrane constituent model functions as well as the cost installation factor (*CI*). *CI* was around 25% of the total capital costs (€) (purchased equipment costs). Therefore, the pipes and valves cost C_{pv} (€), instruments and controls cost C_{IC} , tanks and frames cost C_{TF} , and miscellaneous costs C_{MI} were based on a total membrane area A_m , as represented in the following equations:

$$C_{pv} = 5926.13 A_m^{0.42} \quad (10.1)$$

$$C_{IC} = 1445.5 A_m^{0.66} \quad (10.2)$$

$$C_{TF} = 304721 A_m^{0.53} \quad (10.3)$$

$$C_{MI} = 7865 : 02 A_m^{0.57} \quad (10.4)$$

The membrane and pressure vessel costs were calculated by the multiplication of the membrane and pressure vessel price per unit area (€/m²) by the total membrane area.

The pump cost C_p was calculated based on the total feed flow rate (m³/h) and operating pressure (kPa) as presented in Eq. (10.5):

$$C_p = 622.59(Q_f P)^{0.39} \quad (10.5)$$

The amortisation factor (AF) of the plant was calculated based on the interest rate (i) and the design plant life in years (DL):

$$AF = \frac{i(1+i)^{DL}}{(1+i)^{DL} - 1} \quad (10.6)$$

The amortisation factor of the membrane (AF_m) was calculated based on the mean interest rate of the membrane (i_m) and the membrane lifetime in years (ML):

$$AF_m = \frac{i_m}{(1+i_m)^{ML} - 1} \quad (10.7)$$

The total cost of energy E_c was calculated based on the plant capacity (Q_l) in m³/s, inlet pressure (P_l) in Pa, energy cost (C_e) in €/W h, and pump efficiency and plant permeate flow rate (Q_p) in m³/h.

$$E_c = \frac{Q_l P_l C_e}{\varepsilon_{pump} Q_p} \quad (10.8)$$

The maintenance costs and the pretreatment costs were fixed at 2% of the total investment costs and 15% of the total operating cost minus the maintenance costs.

10.6.3 ECONOMIC RESULTS

The results of this study showed that the total annualised capital cost had the largest contribution in the treatment cost, and which represents around 29.3%. A parametric sensitivity analysis was carried out to explore critical parameters which affect the profitability and the economic indicators of the RO membrane system. These included the plant capacity, number of working hours, feed temperature, recovery ratio, the membrane lifetime, the membrane cost, and the plant design lifetime. The following observations were made:

- The plant capacity, permeate flux, and recovery ratio had the most significant impacts on the total capital cost due to their close relationship to the membrane area.
- The recovered energy of ERD was an important factor for reducing the treatment cost.
- The profitability could be increased by 48.6% as a result of increasing the recovery rate by 20%.

- An improvement of only 3.3% was noticed for the profitability of a longer membrane lifetime.
- The RO process can be profitable after increasing the recovery rate to above 50%.

10.7 ECONOMIC SIMULATION AND OPTIMISATION OF CHLOROPHENOL REMOVAL FROM WASTEWATER

Al-Obaidi et al. (2019) developed a methodology to explore the economic feasibility of retentate and permeate reprocessing strategies in a multi-stage RO process for the removal of chlorophenol from wastewater via simulation and optimisation. A mathematical model (based on the models developed by Al-Obaidi et al. in Chapter 5) was developed to predict the performance of a multi-stage RO process to estimate the total annualised operation cost and product price using an appropriate set of cost functions. A multi-objective non-linear optimisation framework was developed for the process to minimise the product unit cost, total annualised cost, and specific energy consumption. This was carried out while optimising the feed pressure and the feed flow rate with constraints on chlorophenol rejection (90%) and the total water recovery rate (50%). The optimisation framework included the upper and lower limits of several decision variables based on the membrane specifications.

Figure 10.3 shows the proposed schematic diagram of retentate and permeate reprocessing strategies of the proposed configuration of a three-stage RO wastewater treatment connected in series.

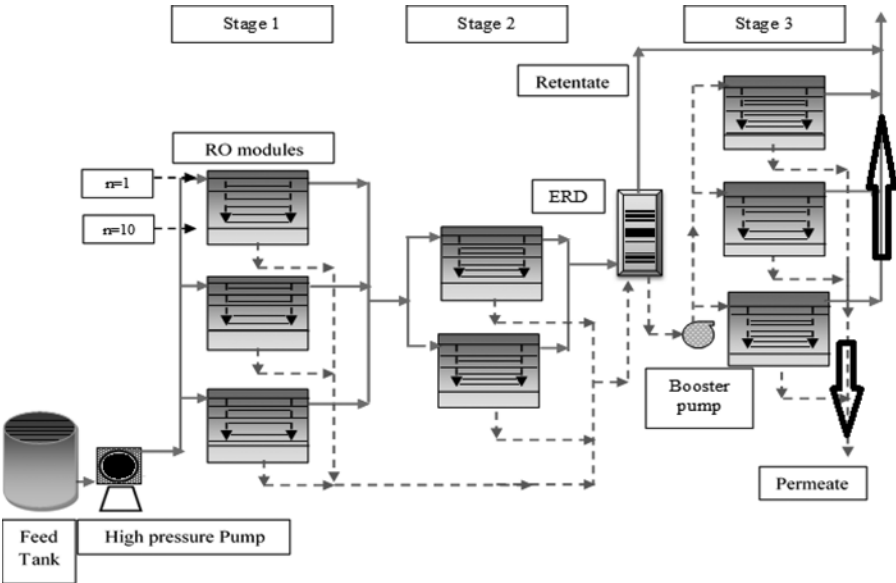


FIGURE 10.3 Schematic diagram of the proposed RO process (80 membrane elements, 1 membrane for each pressure vessel, and 10 membranes in each block).

(Adapted from Al-Obaidi et al., 2019)

10.7.1 PROCESS MODEL DEVELOPMENT

This study adopted the model developed by Al-Obaidi et al. (2018) (based on the models developed by Al-Obaidi et al. in Chapter 5) incorporating the physical property equations relevant to chlorophenol. Several equations were embedded in the process model based on the work of Malek et al. (1996), Marcovecchio et al. (2005), Koroneos et al. (2007), and Lu et al. (2012) to construct the cost model. This included the calculations of operating and capital costs, the wastewater intake and pretreatment cost, the high-pressure pump cost, the booster pump cost, and the energy recovery device cost. The correlation of Koroneos et al. (2007) was considered to estimate the labour and maintenance costs. The calculation of the effluents disposal cost was included in this study. The cost model equations and their descriptions are presented in Table 10.5.

The membrane specification and economic data are given in Table 10.6.

10.7.2 SENSITIVITY ANALYSIS OF OPERATING CONDITIONS

The sensitivity analysis was carried out by measuring the impact of the variation of one operating parameter at a time while other parameters were fixed, on the economic indicators of the multi-stage RO process in terms of the total annualised cost, product unit cost, and specific energy consumption.

The impact of pressure variation at the fixed feed flow rate, concentration and temperature on the total annualised cost, water product cost, specific energy consumption, and total product flow rate is plotted in Figures 10.4 and 10.5, respectively.

Figure 10.4 shows that the total annualised cost increased by around 23% due to the increasing pressure from 13 to 22 atm, which also enhanced the total product flow rate (Figure 10.5). Figure 10.4 shows a reduction of the product unit cost *PUC* by around 13.62% as a response to the pressure change. A noticeable increase in the total product flow rate, around 70.76%, was actually reinforcing the product unit cost (Figure 10.5). Côté et al. (2005) mentioned the possibility of a higher cost saving because of a higher water flux. The product cost actually reduced slowly (beyond 18 atm) as shown in Figure 10.4. Stages 1 and 3 (Figure 10.3) operated at a similar operating pressure. However, increasing the operating pressure in stage 1 required a higher energy and caused an increase in the permeate flow and a reduction in the retentate flow rate entering the ERD and leading to a continuous reduction of the energy recovered by the ERD. To operate stage 3 at the same pressure as stage 1 therefore required a higher energy though the booster pump. Figure 10.5 shows a linear relationship between the operating pressure and the specific energy consumption.

Figure 10.6 shows an increase of the total annualised cost (*TAC*) and the product unit cost (*PUC*) of around 113.9% and 84.78.1%, respectively, as a response to the feed flow rate variation. This is caused by the increasing total capital cost (*TCC*) and operating cost (*TOC*) of around 129.8% and 95.47%, respectively. Increasing the feed flow rate increases the total water flux penetrated through the membrane as a result of decreasing the concentration polarisation. However, a slight increase of around 7.6% is noticed in the product flow rate $Q_{p(plant)}$ due to the feed flow rate variation

TABLE 10.5
The Cost Model of Al-Obaidi et al. (2019)

No.	Correlations	Notes
1	$TAC = TCC + TOC$ $TCC = [(C_{wwip} + C_{Pump} + C_{ERD} + C_{me}) (1.411 \times 0.08)]$ $TOC = OC_{Pu} - OC_{ERD} + OC_{sc} + OC_{ch} + OC_{me} + OC_{lab} + OC_{maint} + OC_{bd}$	The total annualised cost (\$/year) comprises total capital cost and total operational cost
2	$C_{wwip} = 996 (24 \times 3600 Q_{r(plant)})^{0.8}$	The wastewater intake and pretreatment cost (\$) (Malek et al., 1996)
3	$C_{Pump} = \left[52 (3600 Q_{r(plant)}) \left(\frac{P_{r(plant)}}{r_{(Bp)}} 0.101325 \right)^{0.96} \right]$ $+ \left[52 (3600 Q_{r(stage_3)}) \left(\frac{P_{r(Bp)}}{r_{(Bp)}} 0.101325 \right)^{0.96} \right]$ $C_{ERD} = \left[52 (3600 Q_{r(plant)}) \left(\frac{P_{r(plant)}}{r_{(plant)}} 0.101325 \right)^{0.96} \right]$	The capital cost of high-pressure pump, booster pump (\$), and ERD (\$) (Lu et al., 2012)
4	$C_{me} = N_s N_{PV} (C_{ele} N_{ele} + C_{PV})$	The membrane module and pressure vessel capital cost (\$)
5	$OC_{Pu} = 365 \times 24 \left[\left(\frac{(3600 (P_{r(plant)} 0.101325) Q_{r(plant)})}{3.6 \varepsilon_{pump} \varepsilon_{motor}} \right) + \left(\frac{(3600 (P_{r(Bp)} 0.101325) Q_{r(Bp)})}{3.6 \varepsilon_{pump} \varepsilon_{motor}} \right) \right] E_c L_f$	The high-pressure pump and booster pump operating cost (\$/year) and the net operating cost of ERD (expressed in \$/year) (Lu et al., 2012)
6	$OC_{np} = OC_{Pu} - OC_{ERD}$	The annual operating net pumping cost

7		$P_{f(out,ERD)} = (P_{f(out,sys)} \varepsilon_{ERD})$ $P_{f(BP)} = P_{f(plant)} - P_{f(out,ERD)}$	The hydraulic outlet pressures of ERD and booster pump
8		$C_{sc} = 3600 \times 24 \times 365 C_{cf} Q_{p(plant)} L_f$ $OC_{ch} = 3600 \times 24 \times 365 C_{ct} Q_{f(plant)} L_f$ $OC_{bd} = 3600 \times 24 \times 365 C_{bd} Q_{p(plant)} L_f$	The annual operating spares cost (\$/year), annual chemical treatment cost (\$/year), and effluents disposal cost (\$/year)
9		$OC_{me} = 0.2 C_{lab}^{opg}$ $OC_{lab} = C_{lab} \times 24 \times 365 Q_{p(plant)}$	The annual membrane replacement cost (\$/year) and the annual labour cost (\$/year) (Koroneos et al., 2007)
10		$PUC = \frac{\left(\frac{TCC}{CCRF} \right) + TOC}{3600 \times 24 \times 365 Q_{p(plant)}}$ $CCRF = \left[\frac{(i+1)^n - 1}{i(i+1)^n} \right]$ $OC_{main} = 0.02 PUC \times 24 \times 365 Q_{p(plant)}$	The treated water production cost (\$/m³), the capital cost recovery factor (-), and annual maintenance costs (\$/year) (Koroneos et al., 2007)

(Continued)

TABLE 10.5
(Continued)

No.	Correlations	Notes
Total plant specific energy consumption		
11	$SEC = \frac{(P_{f(plant)} \times 101325) Q_{f(plant)}}{Q_{p(Total)} \varepsilon_{pump}} + \frac{((P_{f(mbp)} \times 101325) Q_{f(bp)}) (P_{f(ERD)} \varepsilon_{ERD})}{Q_{p(Total)} \varepsilon_{bp}} - \frac{Q_{p(Total)}}{36E5}$	
<i>Note:</i>		
1.411 and 0.08 in row 1 of Table 10.5 are the site development and indirect costs and the capital charge rate per annum, respectively (Malek et al., 1996). - The two equations of row 2 are specifically applicable for the proposed design of multi-stage RO process of Al-Obaidi et al. (2018). $P_{f(plant)}$, $Q_{f(plant)}$, $Q_{f(stage-3)}$, and $P_{f(bp)}$ in row 3 are the plant pressure, plant volumetric feed flow rate, feed flow rate of stage 3, and the supplied pressure of booster pump, respectively. - The membrane module and pressure vessel capital cost (\$) in row 4 are mainly based on the current membrane and pressure vessel prices. C_{de}, C_{pv}, N_s, N_{de}, and N_{pv} are the membrane element and pressure vessel cost (\$) and the stage, membrane, and pressure vessel numbers, respectively. - The parameters of E_c (\$/kWh) and L_f (-) in row 5 are the electricity unit cost and plant load factor per annum, respectively, which are taken as 0.08 and 0.85 respectively (Marconcchio et al., 2005; Lu et al., 2006; Valladares Linares et al., 2016). ε_{pump}, ε_{bp}, ε_{motor}, ε_{ERD} (-), $P_{f(outERD)}$, $P_{f(out-stage)}$, and $P_{f(bp)}$ (atm, m³/s) are the efficiency of high-pressure pump, booster pump, the motor and ERD, the hydraulic outlet pressure of ERD, retentate pressure of the stage, inlet volumetric flow rate of ERD, and operating pressure of the booster pump, respectively. C_{cp}, C_{cr}, and C_{cd} in row 8 indicate the cost of cartridge filters replacement (0.033 \$/m³), cost of chemical treatment (0.018 \$/m³), and cost of effluents disposal (0.0015 \$/m³), respectively. - The labour cost C_{lab} in row 9 is equal to 0.02 \$/m³. i (-) and n (year) in row 10 are the discount rate and the plant life, respectively. The plant life of 25 years was assumed based on Marconcchio et al. (2005). - The total plant specific energy consumption per cubic metre of permeate in row 11 is calculated in terms of the consumed energy in the high-pressure pump, booster pump, and the recovered energy by the ERD. $P_{f(ERD)}$ and $Q_{f(ERD)}$ are the retentate pressure and retentate flow rate of stage 2, respectively.		

TABLE 10.6
Membrane Characteristics, Design Data, and Cost Parameters

Parameter	Value	Parameter	Value
Supplier	Ion Exchange, India Ltd.	Pump efficiency (ϵ_{pump})	0.85 (–)
$A_{W(Tb)}^*$	9.519E-7 (m/atm s)	Booster pump efficiency ϵ_{Bp}	0.85 (–)
$B_{s(Tb)}$	8.468E-8 (m/s)	ERD efficiency ϵ_{ERD}	0.8 (–)
T_o	31 (°C)	Motor efficiency ϵ_{motor}	0.98 (–)
b^*	8529.45 (atm s/m ⁴)	Discount rate (i)	8% (–)
Effective membrane area (A)	7.85 (m ²)	Plant life (n)	25 (year)
Total membrane area of the plant	627.65 (m ²)	Plant load factor (L_p)	0.85 (–)
Height of the feed spacer (t_p)	0.0008 m	Electricity unit cost (e_c)	0.08 (\$/kWh)
Feed cross section open area (A_s)	0.00672 (m ²)	Membrane element cost (C_{eis})	150 (\$) *
Effective membrane length (L)	0.934 (m)	Pressure vessel cost (C_{PV})	70 (\$) *
Effective membrane width (W)	8.4 (m)	Chemical treatment cost (C_{CT})	0.081 (\$/m ³)
Module diameter	0.0825 (m)	Cartridge filters replacement cost (C_{cf})	0.033 (\$/m ³)
Maximum feed pressure ($P_{f(in)}$)	24.77 (atm)		
Minimum flow rate	1E-4 (m ³ /s)		
Maximum flow rate	1E-3 (m ³ /s)		

* Ion Exchange, India Ltd.
(Adapted from Al-Obaidi et al., 2019)

(Figure 10.7). It was observed that increasing the feed flow rate, which results in a minor rise of the product flow rate, significantly increases the costs. These include the wastewater intake and pretreatment costs, the capital cost of the high-pressure pump, and the capital cost of the ERD, which all lead to a significant increase in the total capital and operating costs.

Figure 10.6 also shows that the product unit cost (PUC) increases with the feed flow rate. Clearly, the product unit cost is inversely proportional to the feed flow rate compared to the operating pressure.

Figure 10.8 shows that the total annualised cost, which decreases by about 4.61% due to the reduction in the total operating cost (TOC) and total capital cost (TCC) around 9.99% and 0.05% respectively, as a response to increasing the operating concentration. Increasing the feed concentration corresponds to a clear reduction in the total product flow rate (Figure 10.9) and the annual spare cost of around 16.23%, a

maintenance cost of around 9%, an annual labour cost of around 16.23%, and a brine disposal cost of around 16.23%. Figure 10.9 also shows the variation of the energy consumption against the operating concentration. This provides an optimum feed concentration, which can be used to minimise the energy consumption.

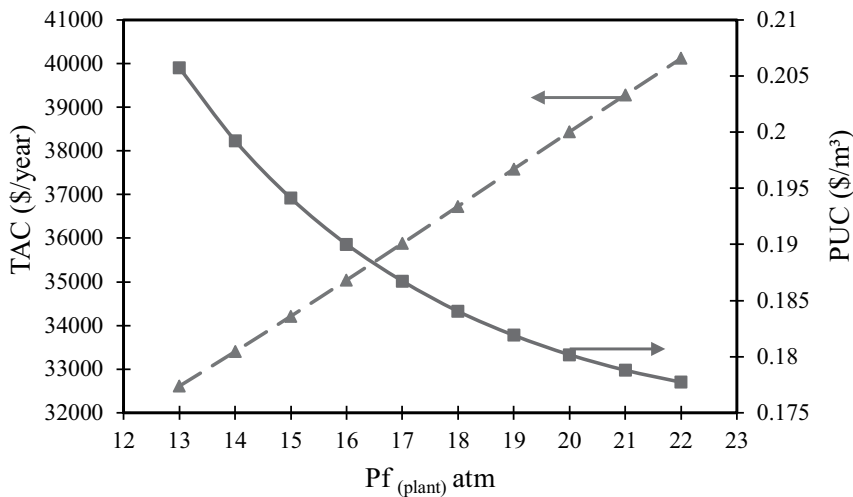


FIGURE 10.4 The total annualised cost and water product unit cost versus the operating pressure (operating conditions: 6.226E-3 kmol/m³, 0.006 m³/s, and 33 °C).

(Adapted from Al-Obaidi et al., 2019)

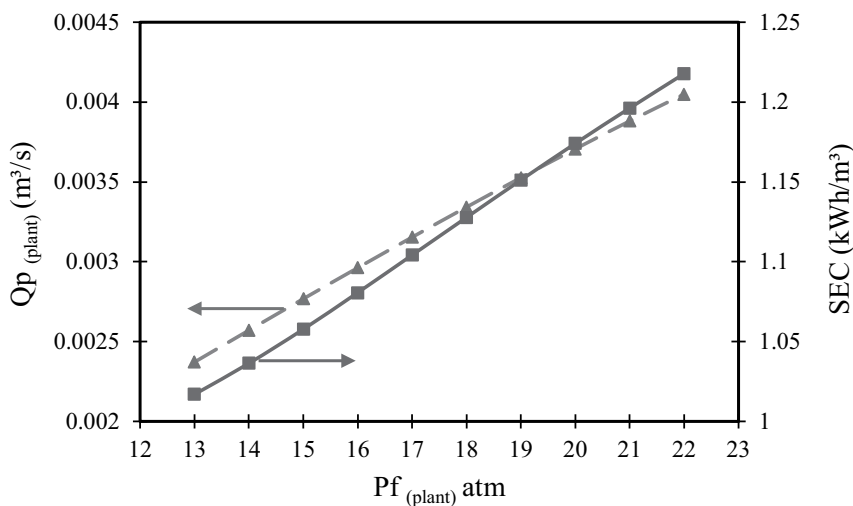


FIGURE 10.5 The product flow rate and specific energy consumption versus the operating pressure (operating conditions: 6.226E-3 kmol/m³, 0.006 m³/s, and 33 °C).

(Adapted from Al-Obaidi et al., 2019)

Figure 10.10 shows an increase in the total annualised cost at around 6.93% due to increasing temperature. Note that the temperature is varied within the regulated limits of the membrane manufacturer and is in line with the industrial effluent conditions.

An increase in total capital cost (TCC) and the total operational cost (TOC) due to increase in the temperature led to an increase in the total annualised cost (TAC). Increasing the capital cost of a high-pressure pump and a booster pump C_{pump} cause an increase in the TCC (as indicated in Eq. 3 in Table 10.5) due to the enhanced feed flow rate of stage 3. Increasing the feed temperature positively impacts the total permeate flow rate and TOC due to a rise of the pumping cost (OC_{pu}), the net pumping cost (OC_{np}), the annual spares cost (OC_{sc}), the effluents disposal cost (OC_{bd}), the annual labour cost (OC_{lab}), and annual maintenance cost (OC_{main}) as can be seen in Eqs. 5, 6, 8(1), 8(3), 9, and 10, respectively, in Table 10.5. Figures 10.10 to 10.12 indicate a reduction of the product unit cost at around 17% as a result of increasing the total product flow rate around 37.7%. Furthermore, increasing the operating temperature decreases the energy consumption at around 13.7% by enhancing the total product flow rate.

Table 10.7 provides the simulation results for the capital and operating costs as well as the performance indicators at the operating conditions. These are 6.226E-3 kmol/m³ for the feed concentration, 0.009 m³/s (777.6 m³/day) for the flow rate, 15 atm for the pressure, and 33 °C for the temperature. A product unit cost of 0.24 (\$/m³) and an energy consumption of 1.44 (kWh/m³) was reported. Figure 10.12 also

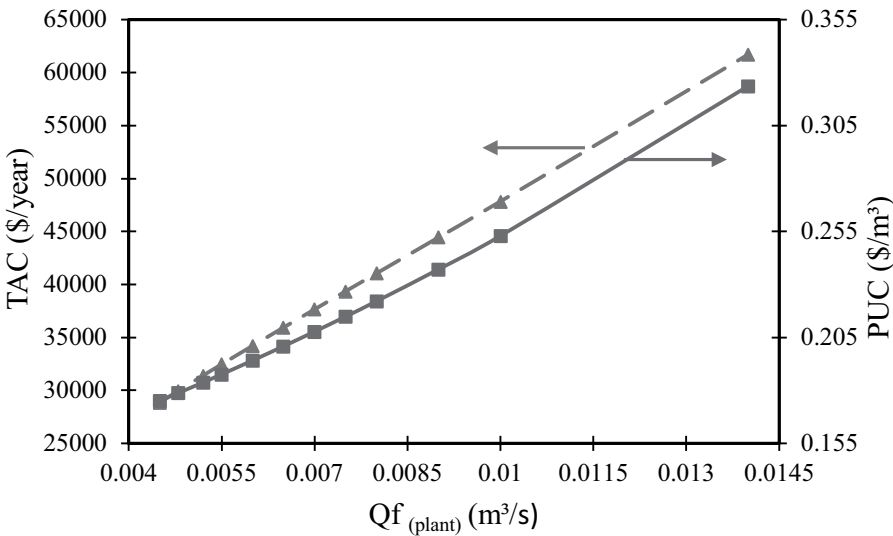


FIGURE 10.6 The total annualised cost and water product unit cost versus the operating feed flow rate (operating conditions: 6.226E-3 kmol/m³, 15 atm, and 33 °C).

(Adapted from Al-Obaidi et al., 2019)

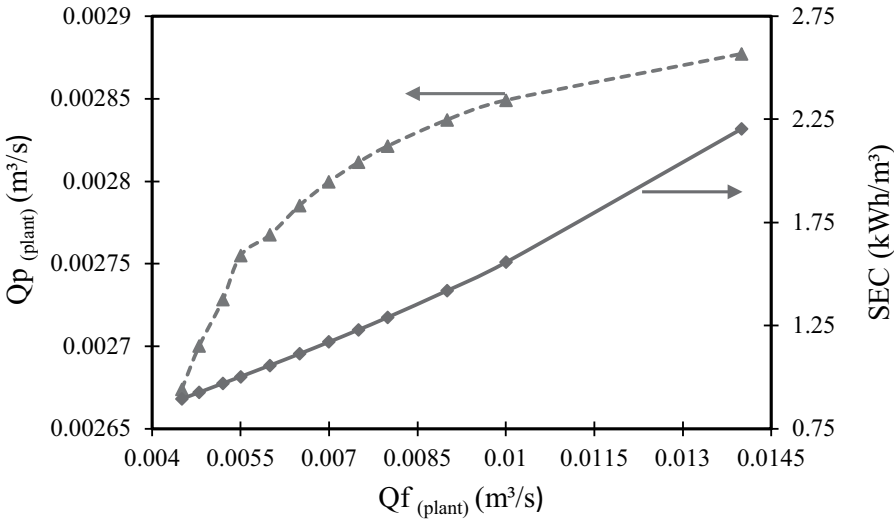


FIGURE 10.7 The product flow rate and specific energy consumption verse the operating feed flow rate (operating conditions: 6.226E-3 kmol/m³, 15 atm, and 33 °C). (Adapted from Al-Obaidi et al., 2019)

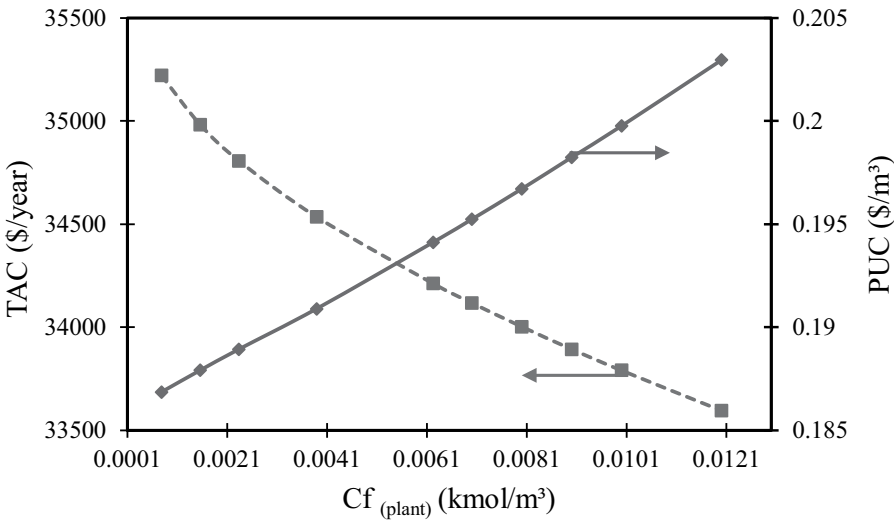


FIGURE 10.8 The total annualised cost and water product unit cost versus the operating concentration (operating conditions: 15 atm, 0.006 m³/s, and 33 °C). (Adapted from Al-Obaidi et al., 2019)

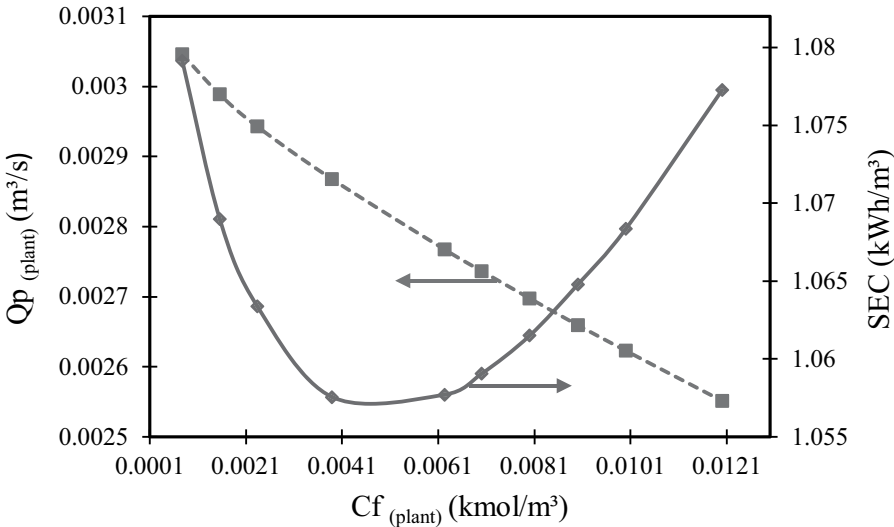


FIGURE 10.9 The product flow rate and specific energy consumption versus the operating concentration (operating conditions: 15 atm, 0.006 m³/s, and 33 °C).

(Adapted with permission from Al-Obaidi et al., 2018)

shows the contribution of the cost parameters on the total annualised cost. This was achieved by calculating the relative ratio of each economic parameter to the total annualised cost. It is evident from Figure 10.12 that the sequence and contribution of the cost elements to the total annualised cost varied quite a bit. Specifically, the annual net pumping cost (OC_{np}) yields the biggest contribution on the total annualised cost, which is also confirmed for an RO seawater desalination (Patroklou and Mujtaba, 2014). Patroklou and Mujtaba (2014) considered a medium-size RO desalination plant of 68 parallel pressure vessels, where each pressure vessel holds only one membrane, and reported a varied contribution of economic parameters on the total annualised cost. They found that the pumping cost had the most dominant impact despite ignoring labour cost calculations.

10.7.3 MULTI-OBJECTIVE OPTIMISATION OF THE RO PROCESS

The multi-objective optimisation problem was built by considering several parameters. These included the chlorophenol rejection and the recovery rate of at least 90% and 50%, respectively. The maximum operating pressure was set at 24.77 atm and the permissible bounds of the feed flow rate of each individual membrane was taken as 1E-4 m³/s to 1E-3 m³/s, and this was selected based on the membrane specifications. The minimum operating temperature was assumed to be 30 °C (same as the experimental work of Sundaramoorthy et al., 2011). However, the medium and maximum operating temperature used were 35 and 40 °C, respectively. Therefore, the optimisation problem had three optimisation sub-problems in line with the three

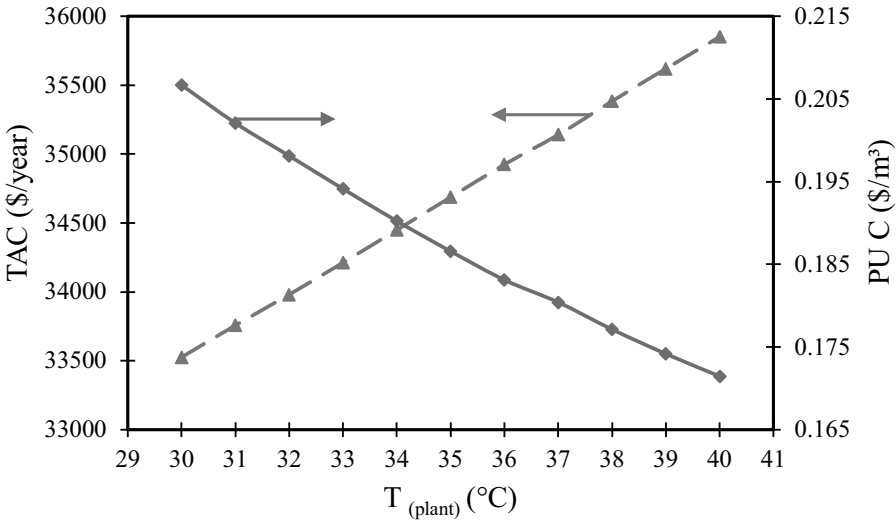


FIGURE 10.10 The total annualised cost and product unit cost versus the operating feed temperature (operating conditions: 6.226E-3 kmol/m³, 15 atm, and 0.006 m³/s). (Adapted from Al-Obaidi et al., 2019)

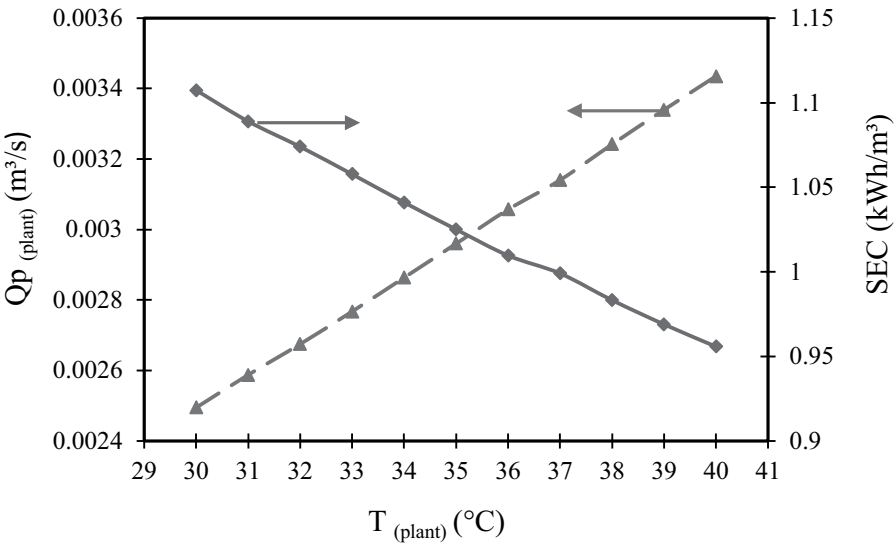


FIGURE 10.11 The product flow rate and specific energy consumption versus the operating feed temperature (operating conditions: 6.226E-3 kmol/m³, 15 atm, and 0.006 m³/s). (Adapted from Al-Obaidi et al., 2019)

TABLE 10.7
Simulation Results of the Proposed Multi-Stage RO Plants

$C_{p(plant)}$ (kmol/ m ³)	$Q_{p(plant)}$ (m ³ /s), (m ³ /day)	$Q_{r(plant)}$ (m ³ /s)	$Rec_{(plant)}$ (–)	$Rej_{(plant)}$ (–)	C_{wwip} (\$)	C_{pump} (\$)	C_{ERD} (\$)	C_{me} (\$)	TCC (\$)	
4.117E-4	2.752E-3 237.77	6.247E-3	0.305	0.933	204580.6	2602.6	2191.1	17600.0	25620.9	
OC_{np} (\$/year)	OC_{sc} (\$/year)	OC_{ch} (\$/year)	OC_{lab} (\$/year)	OC_{me} (\$/year)	OC_{main} (\$/year)	OC_{bd} (\$/year)	TOC (\$/year)	TAC (\$)	PUC (\$/m ³)	SEC (kWh/ m ³)
7155.1	2434.8	4342.5	1736.1	2400.0	420.4	130.20	18619.1	44239.9	0.24	1.44

(Adapted from Al-Obaidi et al., 2019)

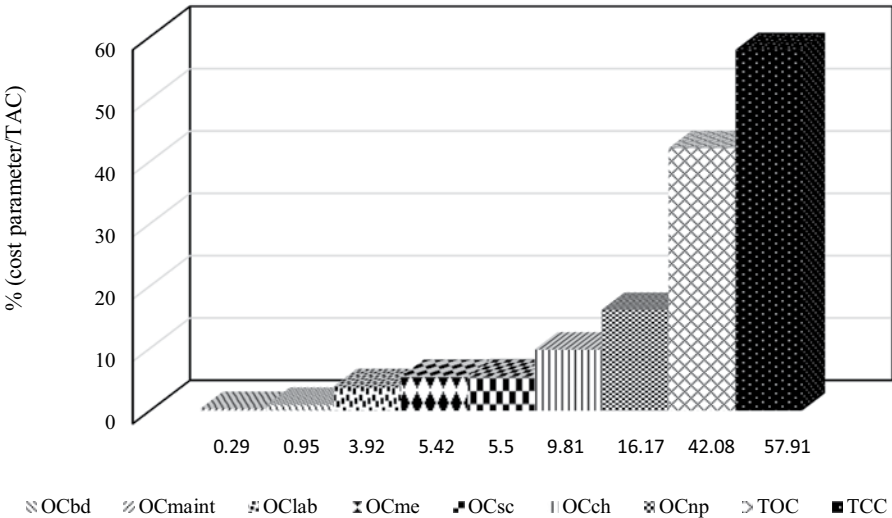


FIGURE 10.12 Cost elements contribution on total annualised cost of the proposed plant.
(Adapted from Al-Obaidi et al., 2019)

industrial effluent temperatures selected. The multi-objective optimisation can be stated as:

Given:

- Feed chlorophenol concentration, feed temperature (30, 35, or 40 °C), module specifications, membrane elements, and pressure vessels number.

Determine:

- Optimal feed pressure and feed flow rate (continuous variables).

So as to:

- Minimise: the product unit cost.
- Minimise: the total annualised cost.
- Minimise: the specific energy consumption.

Subject to:

- Equality (process model) and inequality constraints including the operational parameters of the plant and each membrane element (linear bounds on optimisation variables).

The optimisation problem can therefore be written mathematically as follows:

$$\begin{aligned}
 & \text{Min} \quad \text{PUC} \\
 & \text{Min} \quad \text{TAC} \\
 & \text{Min} \quad \text{S.E.C} \\
 & P_{f(\text{Plant})}, Q_{f(\text{Plant})} \\
 & \text{Subject to:} \\
 & \text{Equality constraints:} \\
 & \text{Process model: } f(x, u, v) = 0 \\
 & \text{Inequality constraints:} \\
 & (10 \text{ atm}) \quad P_{f(\text{plant})}^L \leq P_{f(\text{plant})} \leq P_{f(\text{plant})}^U \cdot (24.771 \text{ atm}) \\
 & (3\text{E-}3 \text{ m}^3/\text{s}) \quad Q_{f(\text{plant})}^L \leq Q_{f(\text{plant})} \leq Q_{f(\text{plant})}^U \cdot (3\text{E-}2 \text{ m}^3/\text{s}) \\
 & \text{Endpoint constraints:} \quad Rec_{(\text{plant})} \geq 50\% \\
 & \quad \quad \quad Rej_{(\text{plant})} \geq 90\% \\
 & T_{(\text{plant})} = 1))30^\circ\text{C}, \quad 2))35^\circ\text{C}, \quad 3))40^\circ\text{C} \\
 & (1\text{E-}4 \text{ m}^3/\text{s}) \quad Q_{f(\text{membrane})}^L \leq Q_{f(\text{membrane})} \leq Q_{f(\text{membrane})}^U \cdot (1\text{E-}3 \text{ m}^3/\text{s})
 \end{aligned}$$

L and U are the lower and upper limits respectively. The optimisation problem was solved using the successive quadratic programming (SQP) method, which is available in the gPROMS software suite.

10.7.3.1 Optimisation Results

The optimisation results are given in Table 10.8.

The optimisation produced the lowest product unit cost and total annualised cost, which should be compared to the simulation results of Table 10.7. Clearly, the operating temperature plays an important role in achieving high recovery, high rejection, low total annualised cost, low energy consumption, and low product cost (40 °C giving the best performance). Minimum recovery and rejection rates were achieved for all cases. It can also be seen that the optimisation had selected lower operating pressures at higher operating temperatures, which helped to minimise the energy consumption. The reduction in the product unit cost was due to the improved water

flux with an increase of the operating temperature. Indeed, these conditions have shown a very promising rejection even at high operating temperatures. The study reported a range of product unit costs from 0.167 to 0.199 \$/m³ and chlorophenol rejection between 90% and 97% for a plant capacity of 202.68 and 292.57 m³/day. The low cost of wastewater treatment compared to seawater desalination is certainly due to the use of a low operating pressure and a low operating concentration, which results in a high recovery rate in the RO wastewater process.

10.7.4 OPTIMUM OPERATING CONDITIONS FOR
MAXIMISING CHLOROPHENOL REJECTION

Al-Obaidi et al. (2019) considered the following non-linear optimisation problem to maximise the rejection for the RO process shown in Figure 10.3.

MinRej_(Plant)
P_{f(Plant)}, Q_{f(Plant)}, T_(Plant)
Subjected to:
Equality constraints:
Process model: f(x, u, v) = 0
Inequality constraints:

$(10\text{ atm})\ P_{f(plant)}^L \leq P_{f(plant)} \leq P_{f(plant)}^U\ (24.771\text{ atm})$
 $(3E-3\text{ m}^3/s)\ Q_{f(plant)}^L \leq Q_{f(plant)} \leq Q_{f(plant)}^U\ (3E-2\text{ m}^3/s)$
 $(30\text{ }^\circ\text{C})\ T_{(plant)}^L \leq T_{(plant)} \leq T_{(plant)}^U\ (40\text{ }^\circ\text{C})$

Endpoint constraints: $Rec_{(plant)} \geq 50\%$

$(1E-4\text{ m}^3/s)\ Q_{f(membrane)}^L \leq Q_{f(membrane)} \leq Q_{f(membrane)}^U\ (1E-3\text{ m}^3/s)$

TABLE 10.8
Optimisation Results of the Proposed Plant at Operating Concentration of 6.226E-3 kmol/m³

T _(Plant) (°C)	Opt Q _{f(Plant)} (m ³ /s) (m ³ /day)	Opt P _{f(Plant)} (atm)	Min PUC (\$/m ³)	Min TAC (\$/ year)	Min SEC (kWh/m ³)	Q _{p(Plant)} (m ³ /s) (m ³ /day)	Rec _(Plant) (–)	Rej _(Plant) (–)
30	6.771E-3 585.01	19.92	0.199	40236.1	1.31	3.386E-3 292.57	0.500	0.900
35	4.303E-3 371.77	13.00	0.173	27116.8	0.80	2.463E-3 212.79	0.572	0.943
40	4.037E-3 348.79	10.80	0.167	25363.9	0.67	2.346E-3 202.68	0.581	0.970

(Adapted from Al-Obaidi et al., 2019)

The optimisation results in Table 10.9 give a maximum chlorophenol rejection of 98.8%. However, the counter effect of the improved chlorophenol rejection is the significant increase in the total annualised cost, energy consumption, and product cost compared to that presented in Table 10.8.

10.8 CONCLUSIONS

Water pollution is ubiquitous in today’s modern and highly industrialised world. This has resulted in a significant increase of random discharges of hazardous compounds into surface water from several industries. Several treatment methods have been developed to remove harmful pollutants from wastewater before releasing the treated water into the environment. Membrane technology has become one of the most feasible and economic solutions for converting wastewater into reusable water commensurate with tighter legislation. Reverse osmosis has been more specifically recognised as one of the most promising technologies for producing safe water for industrial and domestic reuse.

This chapter has provided the state of the art on RO membrane process economics for water and wastewater applications. Several cost functions developed for predicting the water production cost have been discussed and compared. There appears to be a remaining knowledge gap around the economics of product water cost and the associated energy consumption required for RO seawater desalination processes. The existence of toxic chemicals in several industrial effluents and by-products formed during disinfection of oxidation processes continues to pose a realistic challenge. Many such trace concentration chemicals in wastewater require a combination of highly sophisticated treatment methods.

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TABLE 10.9
Optimum Operating Condition of Maximum Chlorophenol Rejection at Feed Concentration of 6.226E-3 kmol/m³

Optimum $Q_{f(plant)}$ (m³/s)	Optimum $P_{f(plant)}$, (atm)	Optimum $T_{(plant)}$ (°C)	$Rec_{(plant)}$ (–)	$Rej_{(plant)}$ (–)	$Q_{p(plant)}$ (m³/s)	PUC, (\$/m³)	TAC, (\$/ year)	SEC, (kWh/m³)
(m³/day)					(m³/day)			
1.198E-2	24.771	40	0.500	0.988	5.987E-3	0.210	68882.73	1.767
1034.98					517.27			

(Adapted from Al-Obaidi et al., 2019)

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Index

Note: Numbers in **bold** indicate tables and numbers in *italic* indicate figures on the corresponding page.

A

- acrylonitrile, 7
- activated carbon adsorption method (ACA), 16–17
- advanced design of a two-stage/two-pass spiral wound RO process for the removal of chlorophenol from wastewater, 333–337
 - optimisation of the two-stage/two-pass spiral wound RO process, 335–337
 - sensitivity analysis, 335
 - two stage/two pass RO process, 333–335
- advanced design of multi-stage RO process for the removal of N-nitrosamine compounds from wastewater, 321–330
 - description of the multi-stage RO process, 322–323
 - model equations, 323–324
 - sensitivity analysis of the operating parameters, 324–330
- advanced oxidation process, 19–20
- advanced treatment methods, 14, 18–21
- aniline (amino benzene), 7, 60, **158**
- application of Genetic Algorithms for optimising an RO desalination process, 305–306
- arsenic, 8, 16, 64, 65–66, 307, **308**

B

- biological treatment methods, 17–18, 21, **24**, 64, 69, 306

C

- cadmium, 8, 64, 65, 66, 307, **308**
- catalytic wet air oxidation (CWAO) process, 20–21
- characteristics of a spiral wound RO process, 41–42
- chromium, 51, 52, 54, 64, 65, 66–68, 71, 257, **308**
- coagulation and flocculation, 15–16, **24**, 45, 56
- comparison of performances by using Model VII and Model VIII, 142
- concentration polarisation theory, 43–44, 94
- configuration of spiral wound module, 42
- the conservation equations of steady state model, 126–127

- the conservation equations of the dynamic model, 124–126
- copper, 8, 25, 51, 54, 64–67, 68, 70–71, 178, 180, 182–183, 182, 398, 402
- cost analysis of an RO process for the reclamation of dairy wastewater
 - economic model of Sethi and Wiesner (2000), 404–405
 - economic results, 405–406
 - RO process description, 404
- cost analysis of RO process for the purification of olive mill wastewater, 402–404
 - economic analysis, 402–404
 - RO process description, 402
- cost evaluation of RO water treatment plants, 401–402
- critique on the modelling of spiral wound reverse osmosis process for wastewater treatment, 171

D

- Dairy wastewater treatment, 58–60
- design and optimisation of membrane elements of a multi-stage RO process for the removal of chlorophenol from wastewater with significant energy savings
 - description of the RO process and feed characteristics, 376
 - impact of changing the height of the feed channel, 378
 - impact of increasing the membrane area by simultaneously increasing membrane length and width, 381
 - impact of membrane area, 378–381
 - impact of membrane dimension on the process performance, 377–378
 - optimisation of RO process configurations with and without an ERD, 381–385
- design and optimisation of the membrane element of a spiral wound RO process for dimethylphenol removal from wastewater at low energy consumption
 - effect of feed channel height, 372

- effect of membrane width and length, 371–372
- optimisation of membrane design parameters, 372–373
- design of a multi-stage RO process for the removal of chlorophenol from wastewater, 322–330
- description of the multi-stage RO process, 322–323
- sensitivity analysis of operating conditions, 324–330
- dynamic simulation: Sensitivity analysis of the operating parameters
 - the removal of chlorophenol from wastewater in an individual spiral wound RO process
 - effect of inlet feed pressure, 239–242
 - effect of inlet feed flow rate, 242–244
 - effect of inlet feed concentration, 244–245
 - removal of dimethylphenol from wastewater in an individual spiral wound RO process, 245–246
 - removal of multiple solutes from a palm oil mill effluent using RO process, 235–239

E

- economic simulation and optimisation of chlorophenol removal from wastewater
 - multi-objective optimisation of the RO process, 415–418
 - optimum operating conditions for maximising chlorophenol rejection, 419–420
 - process model development, 407
 - sensitivity analysis of operating conditions, 407–415
- electroplating wastewater treatment, 54

F

- formulation of an optimisation problem, 264–265, **310**

G

- general concepts of Genetic Algorithm and evolutionary algorithms
 - generalised genetic algorithm, 297–298
 - non-dominated sorting genetic algorithm (NSGA), 299
 - simple genetic algorithm, 298–299
 - species conserving genetic algorithm (SCGA), 299–305

- genetic algorithm optimisation of several industrial wastewater treatment processes, 306
- grand challenges of the world, 1

H

- heavy metals, 1, 8, 16, 18, 21, 23–25, **24**, 53–54, 63–65, 66, 68–71
- highly toxic organic compounds, 4, 7, 8, 26, 73–75, 318
- historical expansion of RO use in wastewater treatment, 49–50, 50
- hollow fibre membrane module, 40, 40, 42, 95
- hybrid systems, 14, 24–26, 53, 57, 72, 269, 273, 275, 306

I

- the importance of simulation studies, 177
- iron, 45, 54, 65, 68–69, 73, 402–403
- irreversible thermodynamic model, 87, 90–95, 101, 158–159, 172, 223, 225

L

- large-scale wastewater system, 61–63
- lead, 8, 24, 54, 64, 65, 69–70
- limitations of conventional treatment methods, 21
- limitations of RO membrane processes, 42–45

M

- membrane fouling, **24**, **42**, 44–45, 65, 70, 306
- membrane technology treatment, 21–23
- membrane transport theories, 90–93
 - irreversible thermodynamic model, 91–93
 - solution diffusion model, 90–91
- mercury, 8, 64–65, 71
- minimisation of freshwater intake in a petroleum refinery Modelling rationale, 276
- minimisation of freshwater intake of pulp and paper processes by recycle and regeneration of wastewater streams, 277–278, 278
- Model I: Al-Bastaki (2004), 95–99
- Model II: Ahmad et al. (2007), 99–104
- Model III: Sagne et al. (2009), 104–108
- Model IV: Srinivasan et al. (2009 and 2010), 108–112
- Model V: Sundaramoorthy et al. (2011a), 112–116
- Model VI: Fujioka et al. (2014), 116–122
- Model VII: Al-Obaidi and Mujtaba (2016), 122–131
- Model VIII: Al-Obaidi et al. (2017b), 131–142
- Model IX: Al-Obaidi et al. (2017c), 142–149
- Model X: Al-Obaidi et al. (2017d), 149–151

- Model XI: Al-Obaidi et al. (2018a), 151–156
 Model XII: Al-Obaidi et al. (2018b), 156–158
 Model XIII: Al-Obaidi et al. (2017e), 159–166
 Model XIV: Al-Obaidi et al. (2017f), 166–171
 multi-stage and multi-pass RO networks
 for the removal of
 N-nitrosodimethylamine -D6
 (NDMA) from wastewater
 multi-stage multi-pass combined permeate
 and retentate reprocessing of an
 RO process, 340–342, 341
 simulation of advanced design of RO
 process, 342
 multi-stage permeate reprocessing design of
 an RO process, 340
 simulation of a permeate reprocessing
 design of an RO process, 340
 multi-stage retentate reprocessing design of
 RO process, 337
 simulation of a retentate reprocessing
 design of an RO process, 337–339,
 338, **339**
- N**
- nanofiltration (NF), 21, 37, **37**, 38, 53, 73, 307,
 394
 nickel, 8, 51, 54, 64–65, 67–68, 70–71, 178,
 182–183, 182
 nitrogenous compounds, 59, 63, 71–73
 NLP-based optimisation, 266–267
 N-nitrosamine, 4, 6–7, 13, 17, 74, 75, 95, 117–119,
 121, 147, 154, 179, 223, 224–226,
 225, 257, 263, 308, 314, 318, 321,
 324–325, 326–328, 327–328, 330
 N-nitrosamine compounds, 74–75, 121, 154, 179,
 223, 308, 314, 318, 330
 N-nitrosodimethylamine (NDMA) removal from
 wastewater, 314–318
- O**
- oily wastewater treatment, 56–57
 optimal RO network configuration for the
 removal of dimethylphenol from
 wastewater, 290–294
 optimisation problem description and
 formulation, 292–293
 optimisation results and discussion, 293–294
 optimal RO network for the removal of phenol
 from wastewater of lube-oil
 recycling plants, 273–275
 optimal RO network for the removal of two
 chlorophenolic compounds from
 pulp wastewater, 270–273
 optimal RO network for the removal of two
 chlorophenolic compounds
 from pulp wastewater using an
 advanced optimisation method,
 275–276
 optimisation of a multi-stage RO process with
 ERD, 330–333
 optimisation of multi-stage multi-pass permeate-
 retentate reprocessing RO process,
 342–344
 Orange County Water District (OCWD): Ground
 water replenishment system in
 California, 61
 overview of membrane processes, 35–36
 overview of RO process modelling for seawater
 and brackish water desalination,
 93–94
 overview of RO process modelling for
 wastewater treatment
 Model I: Al-Bastaki (2004), 95–99
 Model II: Ahmad et al. (2007), 99–104
 Model III: Sagne et al. (2009), 104–108
 Model IV: Srinivasan et al. (2009 and 2010),
 108–112
 Model V: Sundaramoorthy et al. (2011a),
 112–116
 Model VI: Fujioka et al. (2014), 116–122
 Model VII: Al-Obaidi and Mujtaba (2016),
 122–131
 Model VIII: Al-Obaidi et al. (2017b),
 131–142
 Model IX: Al-Obaidi et al. (2017c),
 142–149
 Model X: Al-Obaidi et al. (2017d), 149–151
 Model XI: Al-Obaidi et al. (2018a),
 151–156
 Model XII: Al-Obaidi et al. (2018b), 156–158
 Model XIII: Al-Obaidi et al. (2017e),
 159–166
 Model XIV: Al-Obaidi et al. (2017f),
 166–171
 overview of steady state and dynamic simulations
 of RO wastewater treatment,
 178–179
 overview of the superstructure optimisation for
 a RO processes based wastewater
 treatment, 269–270
 overview of wastewater treatment methods
 advanced treatment methods, 18–21
 advanced oxidation process, 19–20
 catalytic wet air oxidation (CWAO)
 process, 20–21, 20
 biological treatment methods, 17–18
 hybrid systems, 24–26
 limitations of conventional treatment
 methods, 21
 membrane technology treatment, 21–24
 physicochemical treatment methods, 15–17
 activated carbon adsorption method,
 16–17
 coagulation and flocculation, 15–16

P

- parameter estimation using the gPROMS software suite, 145–147
- parameters estimation results, 147
- permeate and retentate streams recycling of
 - multi-stage RO process for chlorophenol removal from wastewater, 344–360
 - description of multi-stage permeate and retentate streams recycling of an RO process, 345
 - impact of the fresh feed flow rate on the performance of a permeate recycling RO process, 357–360
 - sensitivity analysis of operating conditions, 350–357
 - simulation results, 345–350
- pharmaceutical wastewater treatment, 54–56
- phenol and phenolic compounds, 73–74
- physicochemical treatment methods, 15–17, 21, 58
- pilot-scale wastewater system, 60–61
- pollutants
 - N-nitrosamine, 6–7
 - other pollutants, 7
 - Acrylonitrile, 7
 - Aniline (amino benzene), 7
 - phenolic compounds, 5–6
 - pollutants complexity and challenges, 5
- process optimisation
 - formulation of an optimisation problem, 264–265
- pulp and paper wastewater treatment, 57–58

R

- removal of copper from electroplating wastewater in two RO membranes
 - Removal of organic pollutants from wastewater using GA based optimisation
- chlorophenol removal from wastewater, 309–314
 - genetic algorithm parameter setting, 310–312
 - optimisation problem description and formulation, 309–310
 - optimisation results, 312–314
- N-nitrosodimethylamine (NDMA) removal from wastewater, 314–318
 - description of permeate reprocessing multi-stage RO process, 314–315
 - optimisation problem description and formulation, 316
 - optimisation results, 316–318
- removal of specific pollutants from wastewater using RO process

- arsenic, 65–66
- cadmium, 66
- chromium, 66–68
- copper, 68
- heavy metals, 63–65
- highly toxic organic compounds, 73–74
 - phenol and phenolic compounds, 73–74
 - N-nitrosamine compounds, 74
- iron, 68–69
- lead, 69–70
- mercury, 71
- nickel, 70–71
- nitrogenous compounds, 71–73
- reused water: importance and applications, 2–3
- Reverse Osmosis (RO), 38–39
- RO process modelling challenges, 90
- RO process performance measures, 39–40

S

- solution-diffusion model, 87, 89–91, 93–96, 105, 123, 142, 161, 178
- solution of RO optimisation problems, 265–267
 - NLP based optimisation, 266
 - Successive Quadratic Programming (SQP) technique, 266–267
- the sources of wastewater, 2
- spiral wound membrane module, 41–45, 41, 43
- state of the art of economic aspects of water and wastewater RO treatment processes, 390–400
- steady state simulation: sensitivity analysis of the operating parameters
 - removal of a ternary solutes from palm oil mill effluents using RO process, 185–186
 - removal of bisphenol A from wastewater in low-pressure RO process, 190–193
- removal of chlorophenol from wastewater in an individual spiral wound RO process, 193–205
 - feed flow rate, 193–201
 - operating concentration, 203–205
 - operating pressure, 201–203
- removal of copper and nickel from wastewater in a laboratory-scale RO process, 182–183
- removal of copper from electroplating wastewater in two RO membranes, 180–181
- removal of dimethylphenol from wastewater in a multistage RO process, 217–223
 - description of multistage RO configurations, 217
 - RO network performance analysis, 217–223

- removal of dimethylphenol from wastewater in an individual spiral wound RO process, 205–212
- sensitivity analysis, 205–212
- removal of methyl orange dye and Na₂SO₄ salt from wastewater using spiral wound RO process, 183–184
- removal of Nitrosamine from wastewater in a low-pressure RO process, 223–227
- sensitivity analysis of operating conditions, 223–227
- removal of Nitrosamine from wastewater in full-scale multi-stage RO process, 227–235
- removal of phenol from wastewater in an individual spiral wound RO process, 212–217
- removal of phenol from wastewater in SG RO membrane, 186–190
- removal of volatile organic molecules from wastewater using RO process, 186
- superstructure optimisation, 58, 60, 263, 266–269, 277, 290, 401
- superstructure optimisation of the pulp and paper industry using electrodialysis and RO membranes multi-regenerator systems, 284–287
- superstructure optimisation of water network in a petroleum refinery, 278–284

T

- tannery wastewater treatment, 51–52
- textile wastewater treatment, 52–54
- transport mechanisms, 36–37, 90, 172
- types of pressure driven membrane processes, 37–39
 - Nanofiltration (NF), 38
 - Reverse Osmosis (RO), 38–39
- types of RO membrane modules
 - hollow fibre membrane module, 40
 - spiral wound membrane module, 41
 - characteristics of a spiral wound RO process, 41–42
 - configuration of spiral wound module, 42

- limitations of RO membrane processes, 42–45
- concentration polarisation theory, 43–44
- membrane fouling, 44–45

U

- the use of a regenerated water network for optimum water consumption in the dairy industry, 287–290
- use of RO in small to large scale wastewater treatment plants
 - large-scale wastewater system, 61
 - Orange County Water District (OCWD): Ground water replenishment system in California, 61
 - Ulu Pandan (UP) Wastewater Reclamation Plant in Singapore, 61–63
 - pilot-scale wastewater system, 60–61
- use of RO in wastewater treatment in several industrial applications
 - electroplating wastewater treatment, 54
 - dairy wastewater treatment, 58–60
 - oily wastewater treatment, 56–57
 - pharmaceutical wastewater treatment, 54–56
 - pulp and paper wastewater treatment, 57–58
 - tannery wastewater treatment, 51–52
 - textile wastewater treatment, 52–54

V

- variables affecting the water production cost of an RO wastewater treatment, 400–401

W

- wastewater
 - reused water: importance and applications, 2–3
 - the sources of wastewater, 2
 - wastewater and associated challenges, 3–4